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Cr/PCCP-Catalysed Selective Ethylene Oligomerization: Analysis of Various Conformations and the Hemilabile Methoxy Group

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1. Various conformers of catalyst models

CREST was utilized to generate an ensemble of conformers for both catalyst model A and catalyst model B. The initial conformers were fully optimized at the B3LYP/def2-SVP level. The Gibbs free energies of the conformers are summarized in Table S1 and Table S2.

Table S1. Relative Gibbs free energies for various conformers of catalyst model A.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-2730.973951	0.0
2	-2730.973572	0.2
3	-2730.973285	0.4
4	-2730.972866	0.7

Table S2. Relative Gibbs free energies for various conformers of catalyst model B.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-2959.816473	0.0
2	-2959.812889	2.2
3	-2959.812239	2.7
4	-2959.812186	2.7
5	-2959.812085	2.8
6	-2959.811313	3.2
7	-2959.810639	3.7
8	-2959.809774	4.2
9	-2959.809612	4.3
10	-2959.809317	4.5
11	-2959.809058	4.7
12	-2959.809048	4.7
13	-2959.808757	4.8
14	-2959.808466	5.0
15	-2959.808023	5.3
16	-2959.807778	5.5
17	-2959.807462	5.7

2. Spin crossover between two adjacent surfaces

Bis(ethylene) coordinated Cr intermediate 2 is lowest in energy with a sextet spin state. For both catalyst model A and model B, the doublet and quartet spin states are 10 kcal/mol above the sextet state. The transition state of oxidative coupling step is lowest in energy on the quartet surfaces. For both catalyst model A and catalyst model B, the doublet and sextet spin states are 20 kcal/mol above the quartet state. The reaction is greatly promoted by spin surface crossing between the sextet surface and the quartet surface, which effectively reduces the reaction energy barrier.

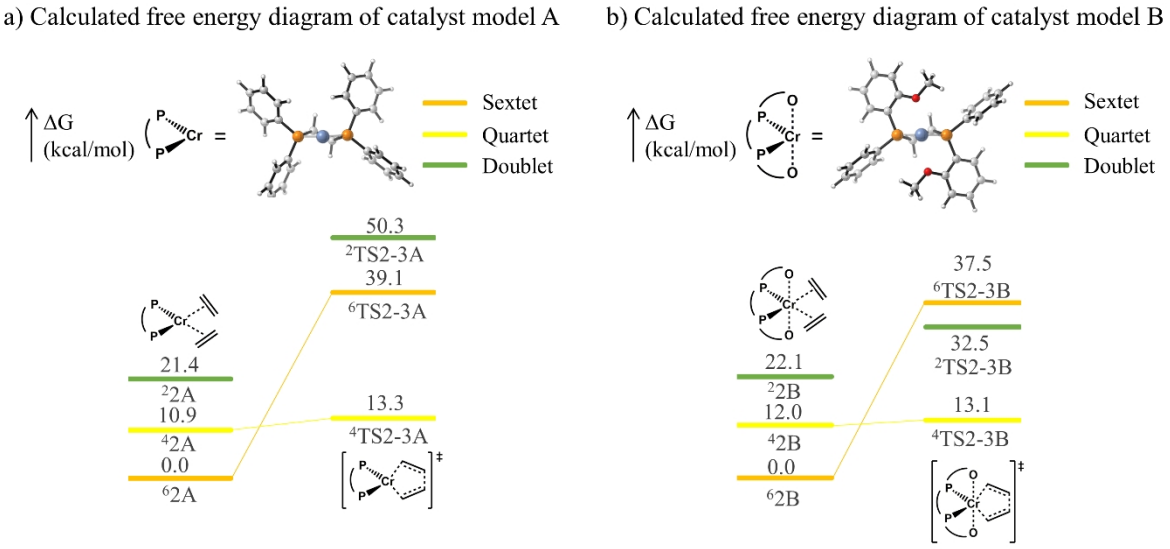

Fig. S1. Calculated free energy diagram. The relative Gibbs free energies calculated at M06L-D3/def2-TZVP//B3LYP-D3/def2-SVP level are given in kcal/mol. The doublet, quartet, and sextet surfaces are depicted in green, yellow and orange, respectively. The superscript numbers (2,4,6) refer to the spin multiplicity.

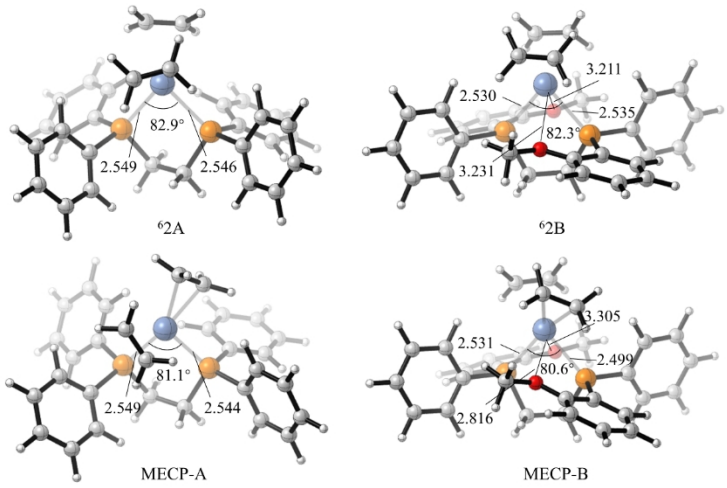

Fig. S2. Geometries of MECPs (Bottom) and bis(ethylene)Cr complex (Top) of catalyst model A (Left) and catalyst model B (Right).

3. Formation of 1-butene by ethylene dimerization

Starting from the intermediate chromacyclopentane ^{4}3, there are two paths. One is the two-step hydrogen transfer to form 1-butene, and the second is the formation of the chromacycloheptane by migratory insertion of the third ethylene molecule. The formation of 1-butene requires to overcome a high energy barrier (^{4}3→^{4}TS7-8) of 19.4 kcal/mol for catalyst model A, and 27.3 kcal/mol for catalyst model B. So, the intermediate chromacyclopentane favors expansion to form chromacycloheptane rather than elimination to yield 1-butene.

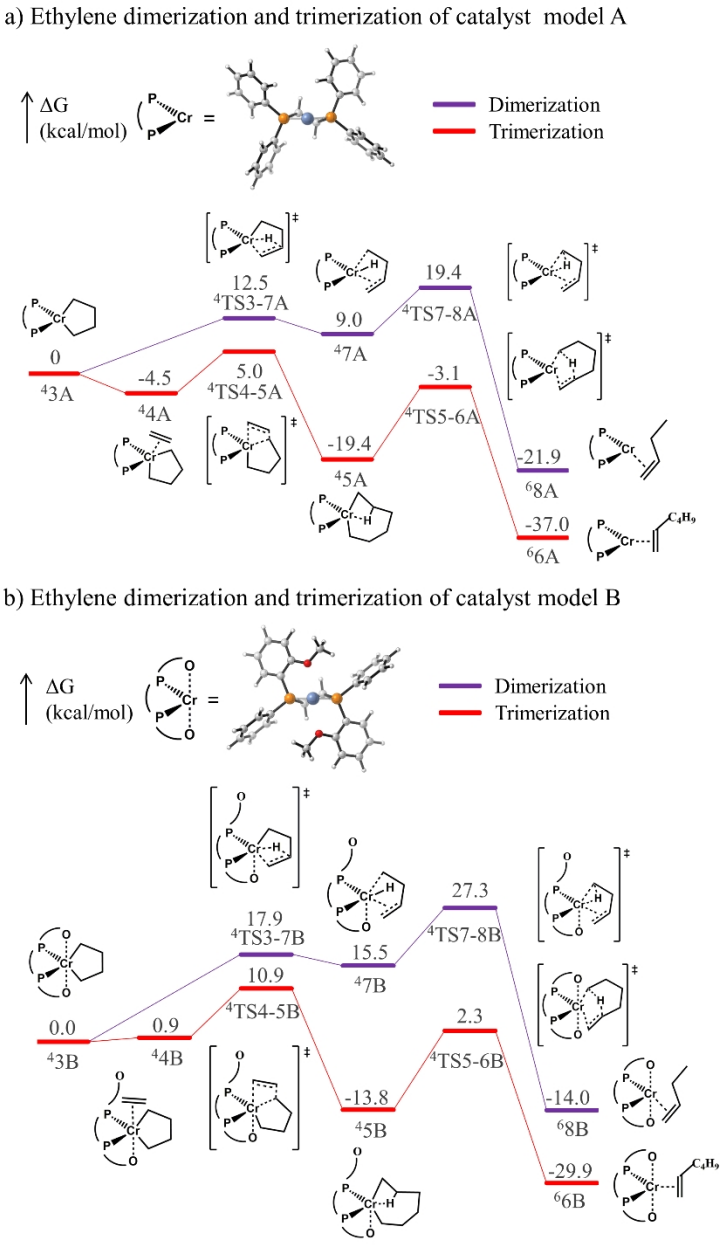

Fig. S3. Calculated free energy diagram for ethylene dimerization and trimerization of catalyst model A and catalyst model B. The relative Gibbs free energies calculated at M06L-D3/def2-TZVP//B3LYP-D3/def2-SVP level are given in kcal/mol. The superscript number (4,6) refer to the spin multiplicity.

4. Various conformers of transition state TS5-6

TS5-6 is one of the key transition states for the selective tri-/tetramerization of ethylene according to the metallacycle mechanism. CREST was utilized to generate an ensemble of conformers for the transition state TS5-6A and TS5-6B, respectively. The initial conformers were fully optimized at the B3LYP/def2-SVP level. The Gibbs free energies of the conformers are summarized in Table S3 and Table S4. The graphical representations of the conformers of TS5-6 of catalyst model A and catalyst model B are shown in Fig. S4 and Fig. S5, respectively.

Table S3. Relative Gibbs free energies for various conformers of ^{4}TS5-6A.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-2966.498635	0.0
2	-2966.496760	1.2
3	-2966.495768	1.8
4	-2966.492243	4.0
5	-2966.491981	4.2
6	-2966.490994	4.8

Table S4. Relative Gibbs free energies for various conformers of ^{4}TS5-6B.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-3195.346518	0.0
2	-3195.346449	0.0
3	-3195.345927	0.4
4	-3195.343531	1.9
5	-3195.343520	1.9
6	-3195.342927	2.3
7	-3195.342469	2.5
8	-3195.342159	2.7
9	-3195.341694	3.0
10	-3195.341631	3.1
11	-3195.341178	3.4
12	-3195.340676	3.7

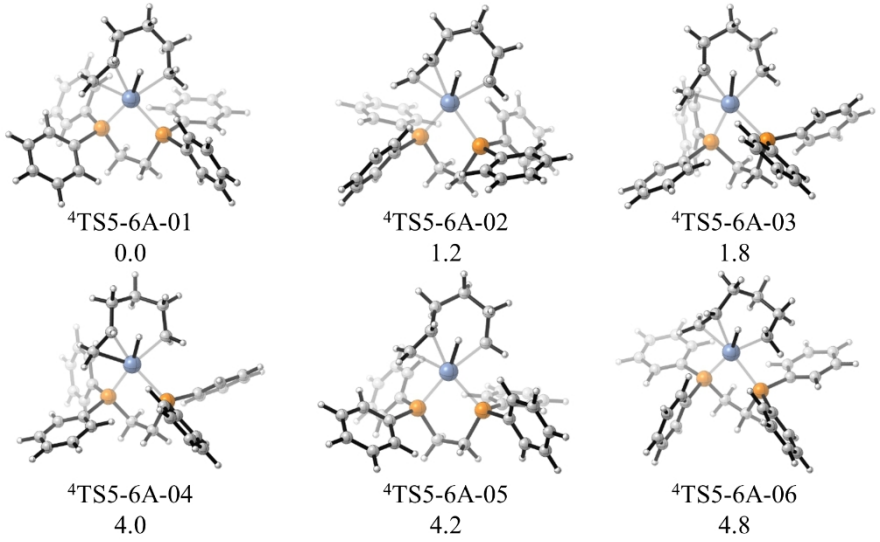

Fig. S4. Graphical representations of the conformers of TS5-6 of catalyst model A. The Gibbs free energies (kcal/mol) relative to the lowest TS5-6A are also shown.

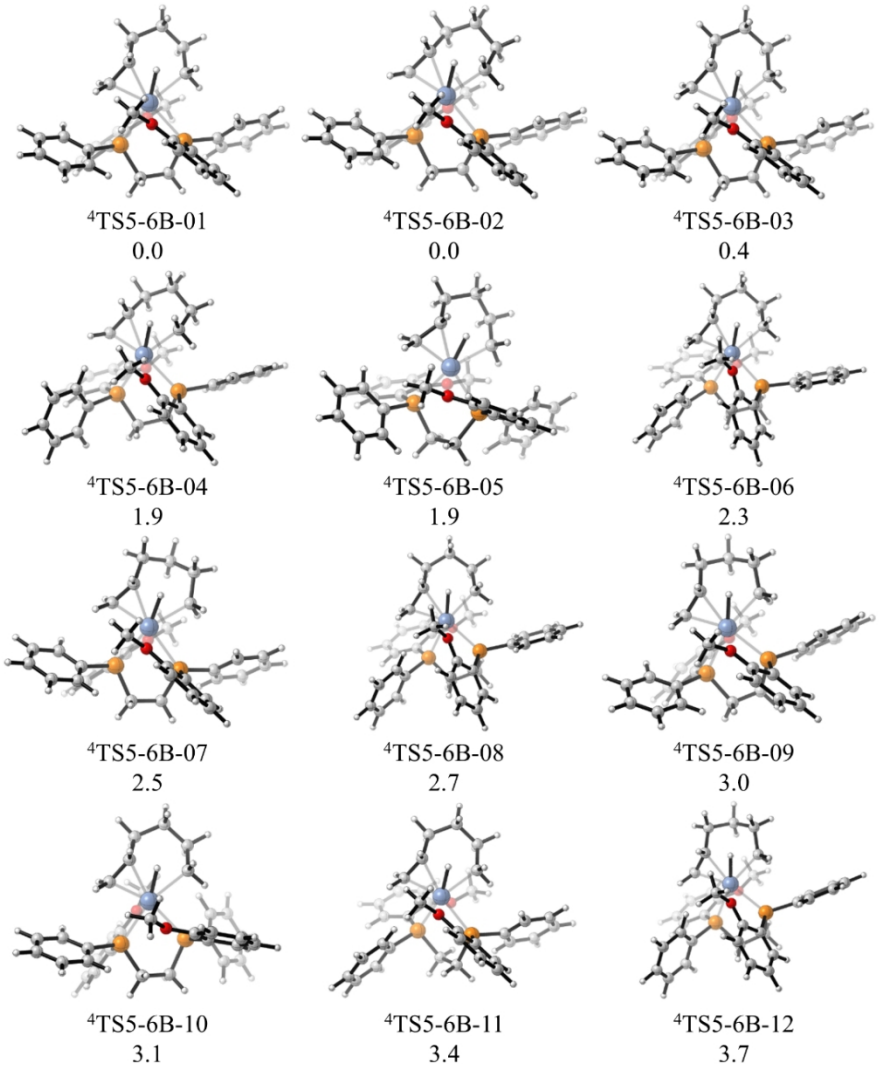

Fig. S5. Graphical representations of the conformers of TS5-6 of catalyst model B. The Gibbs free energies (kcal/mol) relative to the lowest TS5-6B are also shown.

5. Various conformers of transition state TS9-10

TS9-10 is another key transition state for the selective tri-/tetramerization of ethylene according to the metallacycle mechanism. CREST was utilized to generate an ensemble of conformers for the transition state TS9-10A and TS9-10B, respectively. The initial conformers were fully optimized at the B3LYP/def2-SVP level. The Gibbs free energies of the conformers are summarized in Table S5 and Table S6. The graphical representations of the conformers of TS9-10 of catalyst model A and catalyst model B are shown in Fig. S6 and Fig. S7, respectively.

Table S5. Relative Gibbs free energies for various conformers of ^{4}TS9-10A.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-3044.999209	0.0
2	-3044.996666	1.6
3	-3044.996538	1.7
4	-3044.996266	1.9
5	-3044.996205	1.9
6	-3044.996198	1.9
7	-3044.994598	2.9
8	-3044.99423	3.1
9	-3044.993681	3.5
10	-3044.993433	3.6
11	-3044.99261	4.1
12	-3044.992583	4.2
13	-3044.991932	4.6
14	-3044.991837	4.6
15	-3044.991634	4.8
16	-3044.991492	4.8
17	-3044.991358	4.9
18	-3044.991169	5.1
19	-3044.988736	6.6
20	-3044.986738	7.8
21	-3044.981416	11.2

Table S6. Relative Gibbs free energies for various conformers of ^{4}TS9-10B.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-3273.844406	0.0
2	-3273.842082	1.5
3	-3273.841173	2.0
4	-3273.841132	2.1
5	-3273.840341	2.6
6	-3273.840334	2.6
7	-3273.840230	2.6
8	-3273.839354	3.2
9	-3273.839204	3.3
10	-3273.838729	3.6
11	-3273.838617	3.6
12	-3273.838435	3.7
13	-3273.838250	3.9
14	-3273.838050	4.0
15	-3273.837710	4.2
16	-3273.837632	4.3
17	-3273.837405	4.4
18	-3273.837341	4.4
19	-3273.836869	4.7
20	-3273.836611	4.9
21	-3273.836206	5.1
22	-3273.835116	5.8
23	-3273.834976	5.9
24	-3273.834670	6.1
25	-3273.834326	6.3

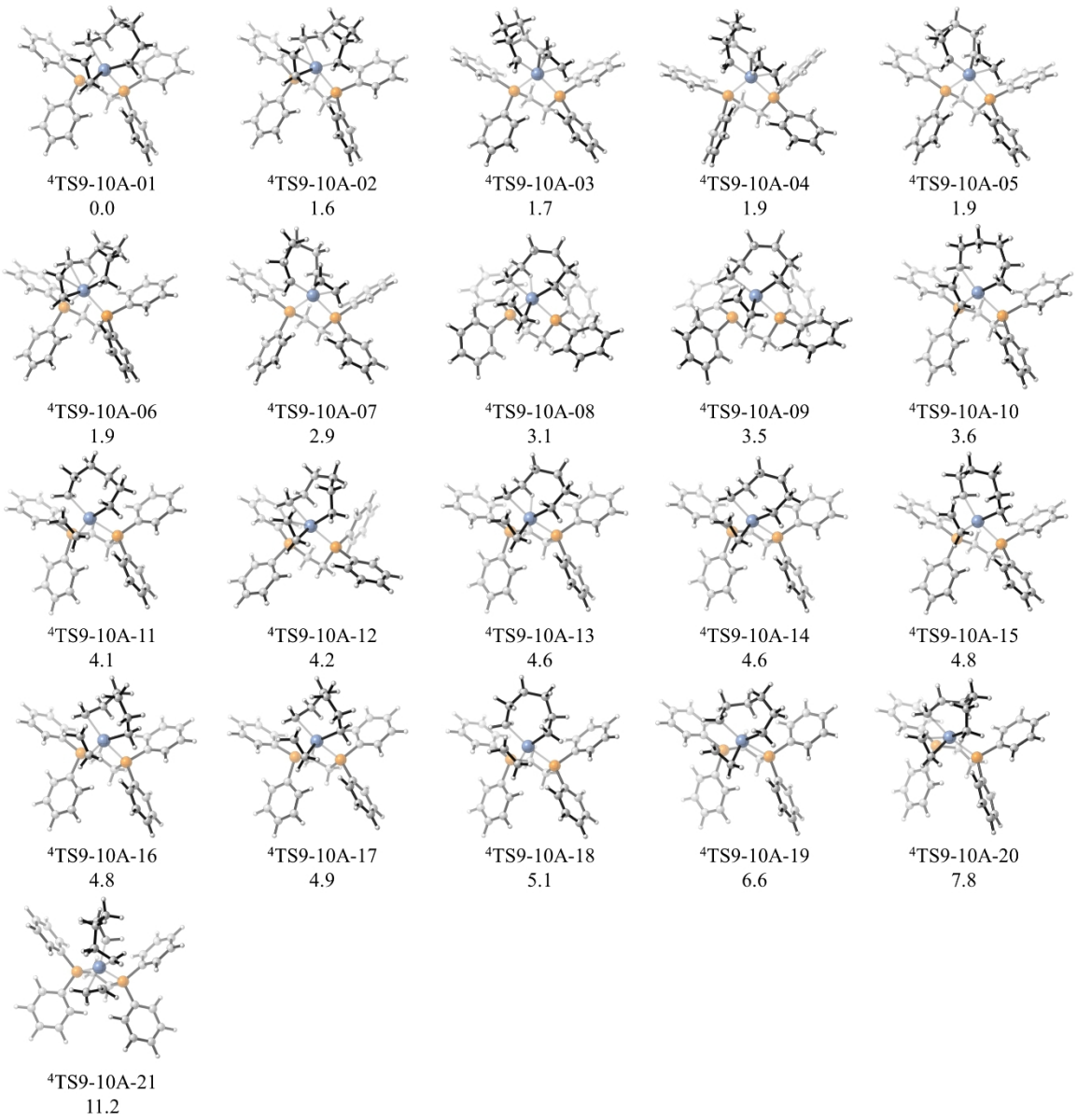

Fig. S6. Graphical representations of the conformers of TS9-10 of catalyst model A. The Gibbs free energies (kcal/mol) relative to the lowest TS9-10A are also shown.

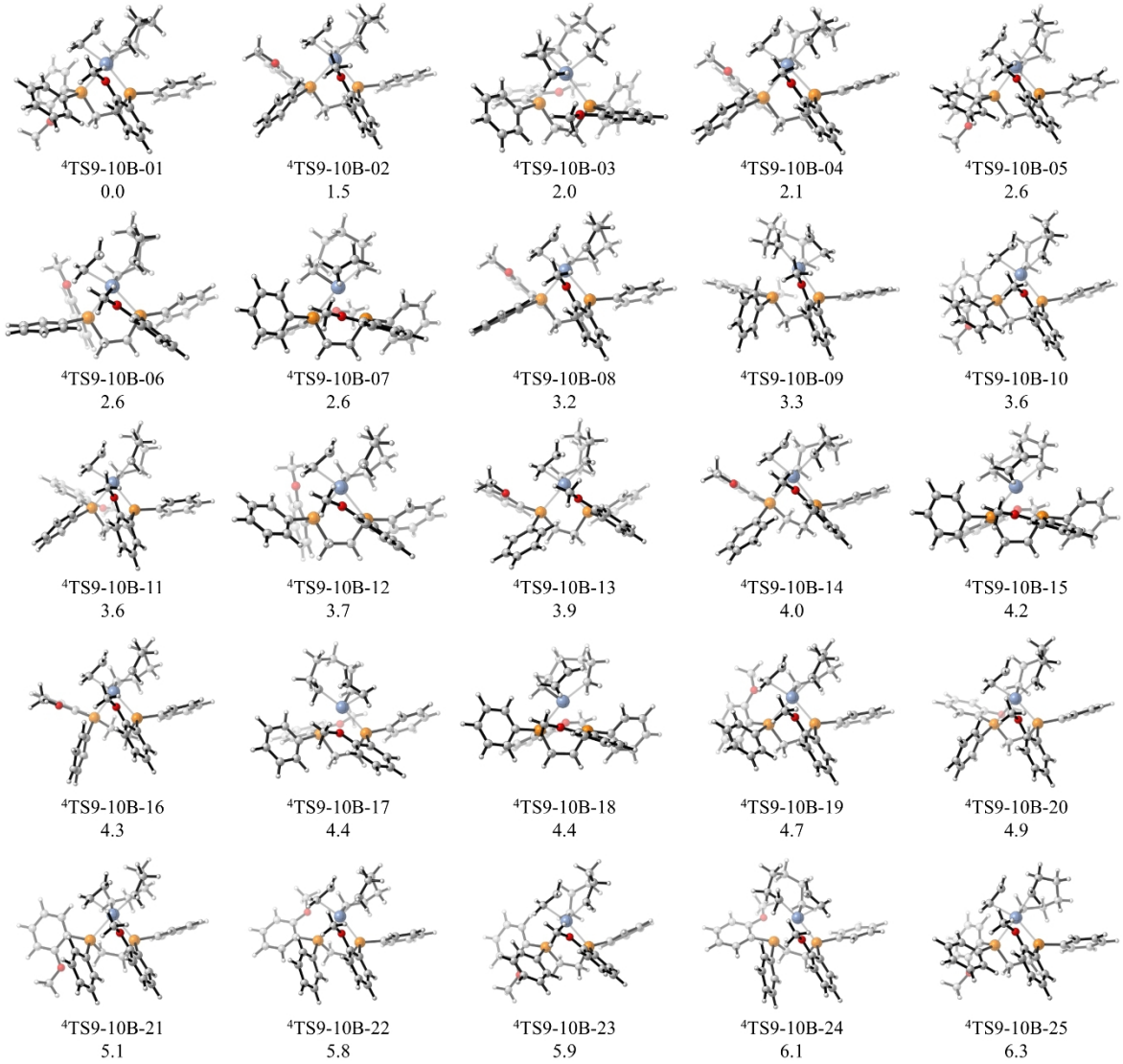

Fig. S7. Graphical representations of the conformers of TS9-10 of catalyst model B. The Gibbs free energies (kcal/mol) relative to the lowest TS9-10B are also shown.

6. Various conformers of the key intermediates chromacyclopentane (3), chromacycloheptane (5), and chromacyclononane (10)

Chromacyclopentane (3), chromacycloheptane (5), and chromacyclononane (10) are key intermediates for the selective tri-/tetramerization of ethylene according to the metallacycle mechanism. CREST was utilized to generate an ensemble of conformers for the key intermediates chromacyclopentane (3), chromacycloheptane (5), and chromacyclononane (10) of catalyst model A and catalyst model B, respectively. The initial conformers were fully optimized at the B3LYP/def2-SVP level. The Gibbs free energies of the conformers are summarized in Table S7-S12.

Table S7. Relative Gibbs free energies for various conformers of chromacyclopentane ^{4}3A.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-2887.989351	0.0
2	-2887.987581	1.1
3	-2887.987504	1.2
4	-2887.987011	1.5
5	-2887.986810	1.6
6	-2887.986574	1.7
7	-2887.986567	1.7
8	-2887.986352	1.9
9	-2887.986281	1.9
10	-2887.986063	2.1
11	-2887.985556	2.4
12	-2887.985346	2.5
13	-2887.984688	2.9
14	-2887.984081	3.3
15	-2887.983908	3.4
16	-2887.983907	3.4
17	-2887.982647	4.2
18	-2887.980245	5.7
19	-2887.976619	8.0

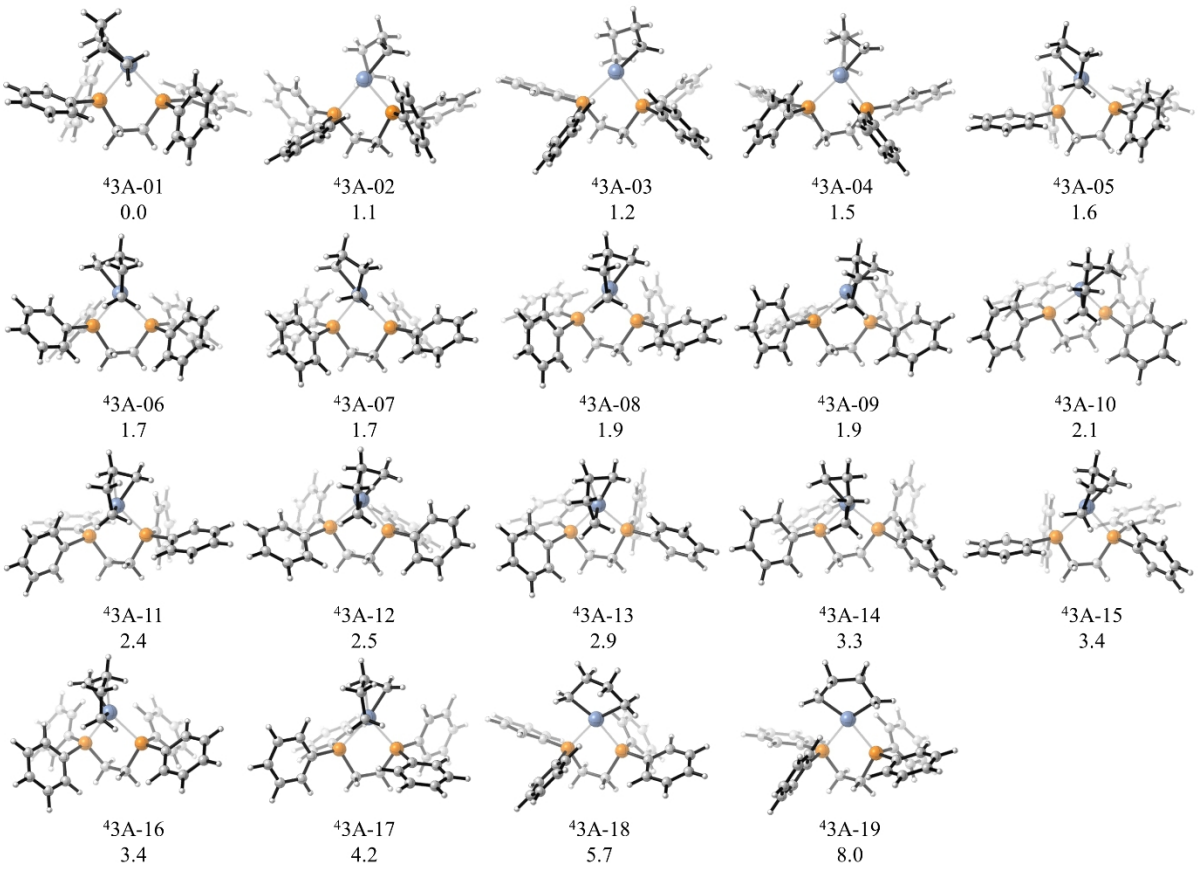

Fig. S8. Graphical representations of the conformers of ^{4}3 of catalyst model A. The Gibbs free energies (kcal/mol) relative to the lowest ^{4}3A are also shown.

Table S8. Relative Gibbs free energies for various conformers of chromacycloheptane ^{4}5A.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-2966.523013	0.0
2	-2966.522824	0.1
3	-2966.521870	0.7
4	-2966.521741	0.8
5	-2966.521391	1.0
6	-2966.521285	1.1
7	-2966.521284	1.1
8	-2966.520884	1.3
9	-2966.520370	1.7
10	-2966.519920	1.9
11	-2966.518903	2.6
12	-2966.517417	3.5

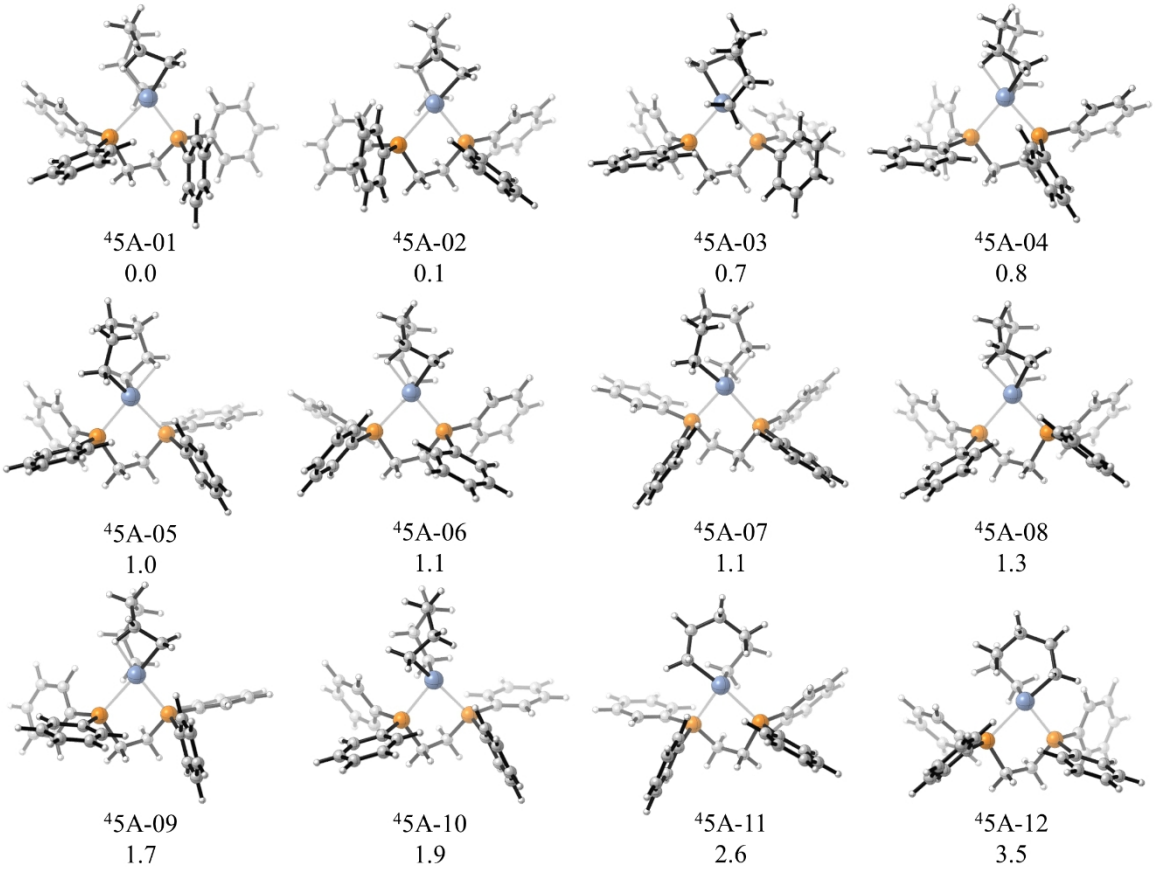

Fig. S9. Graphical representations of the conformers of ^{4}5 of catalyst model A. The Gibbs free energies (kcal/mol) relative to the lowest ^{4}5A are also shown.

Table S9. Relative Gibbs free energies for various conformers of chromacyclononane [4]10A.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-3045.044339	0.0
2	-3045.044121	0.1
3	-3045.043507	0.5
4	-3045.042668	1.0
5	-3045.042422	1.2
6	-3045.042398	1.2
7	-3045.042074	1.4
8	-3045.042030	1.4
9	-3045.041961	1.5
10	-3045.041599	1.7
11	-3045.041582	1.7
12	-3045.041358	1.9
13	-3045.041126	2.0
14	-3045.040805	2.2
15	-3045.040264	2.6
16	-3045.040168	2.6
17	-3045.039878	2.8
18	-3045.039729	2.9
19	-3045.039481	3.0
20	-3045.038872	3.4
21	-3045.038187	3.9
22	-3045.038132	3.9
23	-3045.038047	3.9
24	-3045.037388	4.4
25(10')	-3045.034126	6.4

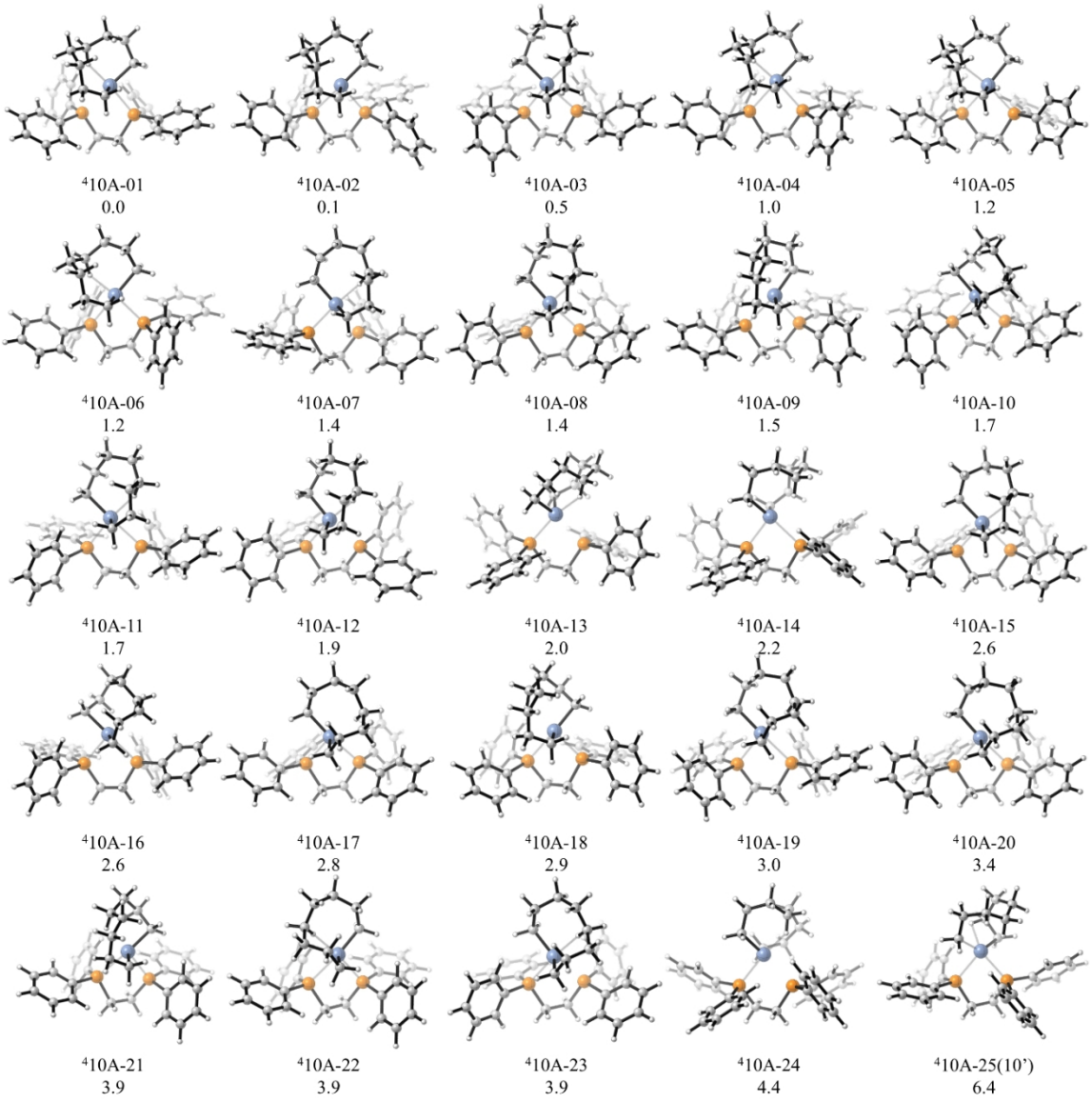

Fig. S10. Graphical representations of the conformers of ^{4}10 of catalyst model A. The Gibbs free energies (kcal/mol) relative to the lowest ^{4}10A are also shown.

Table S10. Relative Gibbs free energies for various conformers of chromacyclopentane ^{4}3B.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-3116.848140	0.0
2	-3116.848026	0.1
3	-3116.846313	1.1
4	-3116.845426	1.7
5	-3116.844345	2.4
6	-3116.843608	2.8
7	-3116.843050	3.2
8	-3116.841953	3.9
9	-3116.841032	4.5
10	-3116.833718	9.0

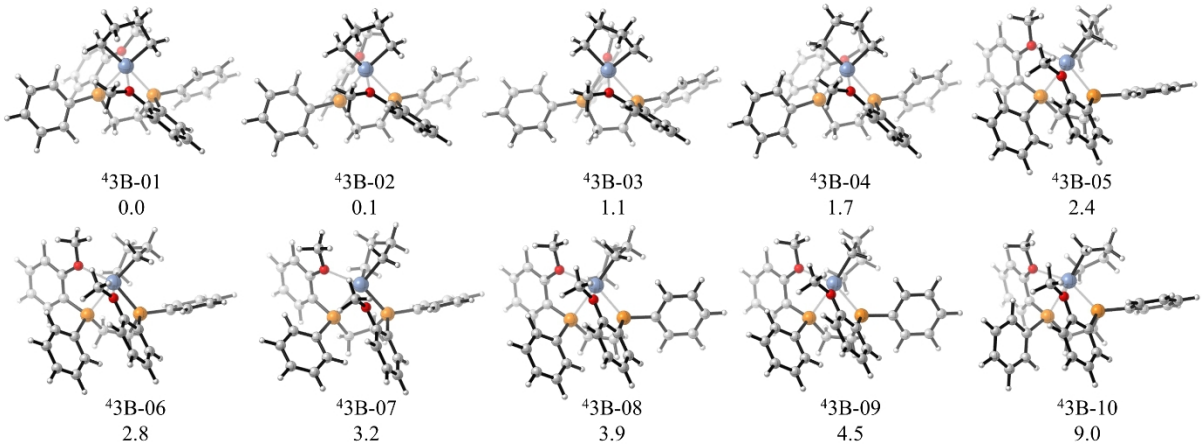

Fig. S11. Graphical representations of the conformers of ^{4}3 of catalyst model B. The Gibbs free energies (kcal/mol) relative to the lowest ^{4}3B are also shown.

Table S11. Relative Gibbs free energies for various conformers of chromacycloheptane ^{4}5B.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-3195.370743	0.0
2	-3195.370432	0.2
3	-3195.370095	0.4
4	-3195.369962	0.5
5	-3195.369846	0.6
6	-3195.369083	1.0
7	-3195.368791	1.2
8	-3195.368731	1.3
9	-3195.368419	1.5
10	-3195.368264	1.6
11	-3195.367038	2.3
12	-3195.367027	2.3
13	-3195.365565	3.2
14	-3195.365216	3.5
15	-3195.364929	3.6
16	-3195.364074	4.2
17	-3195.363751	4.4
18	-3195.363255	4.7
19	-3195.361717	5.7

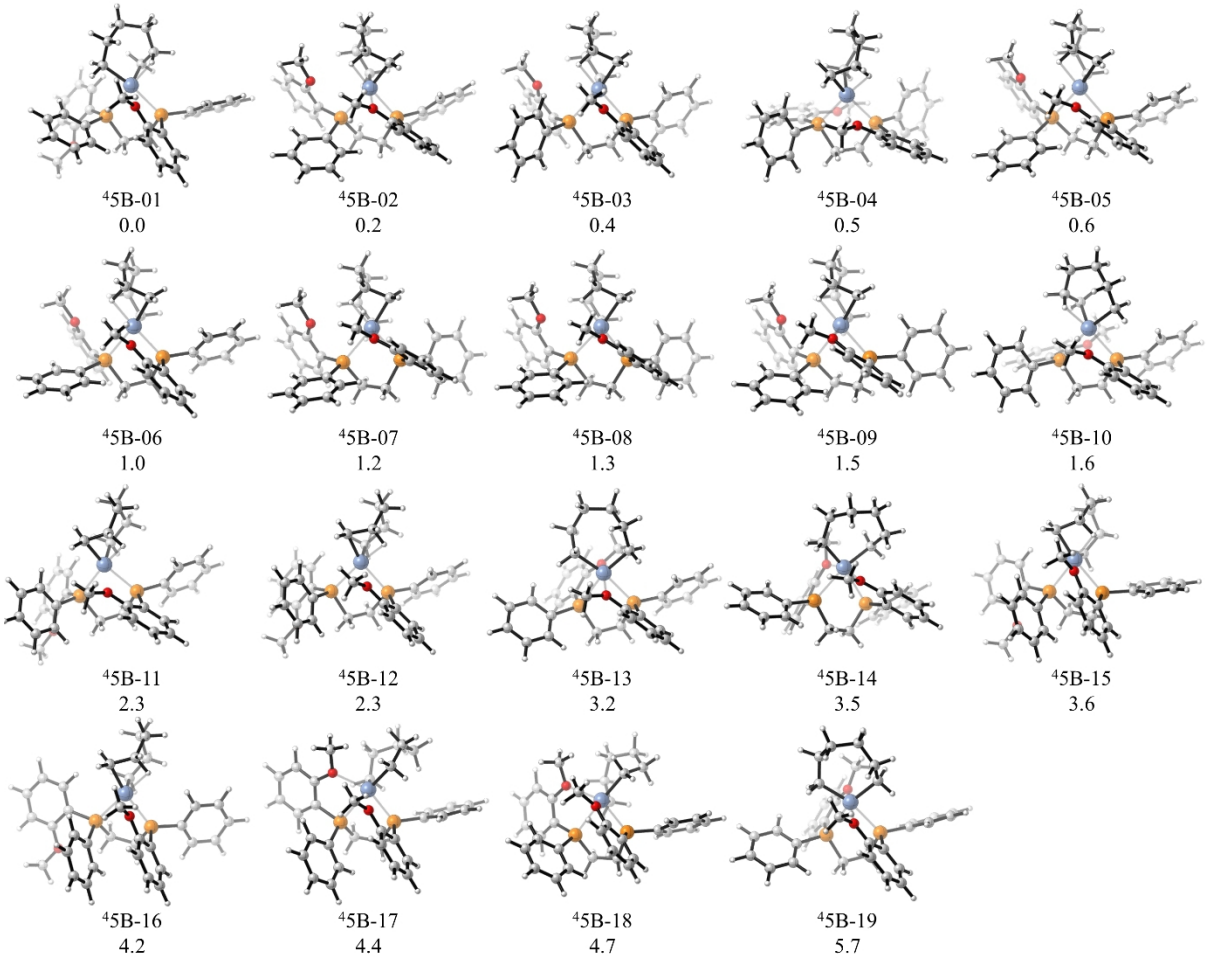

Fig. S12. Graphical representations of the conformers of ^{4}5 of catalyst model B. The Gibbs free energies (kcal/mol) relative to the lowest ^{4}5B are also shown.

Table S12. Relative Gibbs free energies for various conformers of chromacyclononane ^{4}10B.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-3273.888786	0.0
2	-3273.888655	0.1
3	-3273.888159	0.4
4	-3273.887907	0.6
5	-3273.887820	0.6
6	-3273.887312	0.9
7	-3273.886331	1.5
8	-3273.885748	1.9
9	-3273.885241	2.2
10	-3273.885141	2.3
11	-3273.884590	2.6
12	-3273.884517	2.7
13	-3273.884479	2.7
14	-3273.883324	3.4
15	-3273.882991	3.6
16	-3273.882683	3.8
17(10')	-3273.882573	3.9
18	-3273.882536	3.9
19	-3273.881614	4.5
20	-3273.881083	4.8

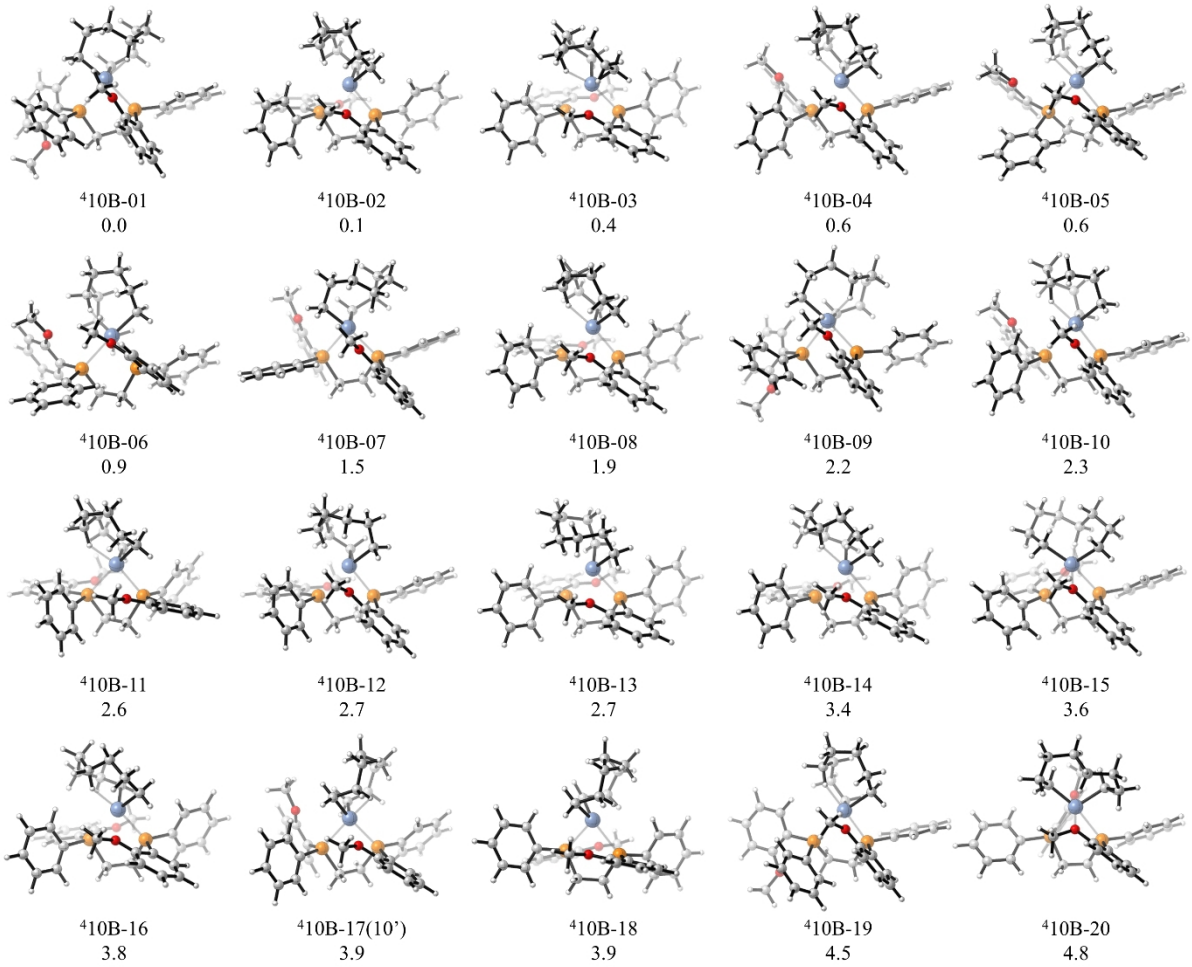

Fig. S13. Graphical representations of the conformers of ^{4}10 of catalyst model B. The Gibbs free energies (kcal/mol) relative to the lowest ^{4}10B are also shown.

7. Various conformers of the ethylene-coordinated complex 9

The ethylene-coordinated complex 9 is of crucial importance to investigate the role of the hemilabile methoxy group. CREST was utilized to generate an ensemble of conformers for the intermediate 9 of catalyst model A and catalyst model B, respectively. The initial conformers were fully optimized at the B3LYP/def2-SVP level. The Gibbs free energies of the conformers are summarized in Table S13 and Table S14.

Table S13. Relative Gibbs free energies for various conformers of ^{4}9A.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-3045.023605	0.0
2	-3045.023153	0.3
3	-3045.022805	0.5
4	-3045.022410	0.7
5	-3045.022071	1.0
6	-3045.021911	1.1
7	-3045.021514	1.3
8	-3045.020850	1.7
9	-3045.019616	2.5
10	-3045.018788	3.0
11	-3045.017928	3.6
12	-3045.017824	3.6
13	-3045.017620	3.8
14	-3045.017426	3.9
15	-3045.017174	4.0
16	-3045.016591	4.4
17	-3045.016236	4.6
18	-3045.016122	4.7
19	-3045.016014	4.8
20	-3045.015868	4.9
21	-3045.015361	5.2
22	-3045.015299	5.2
23	-3045.014319	5.8

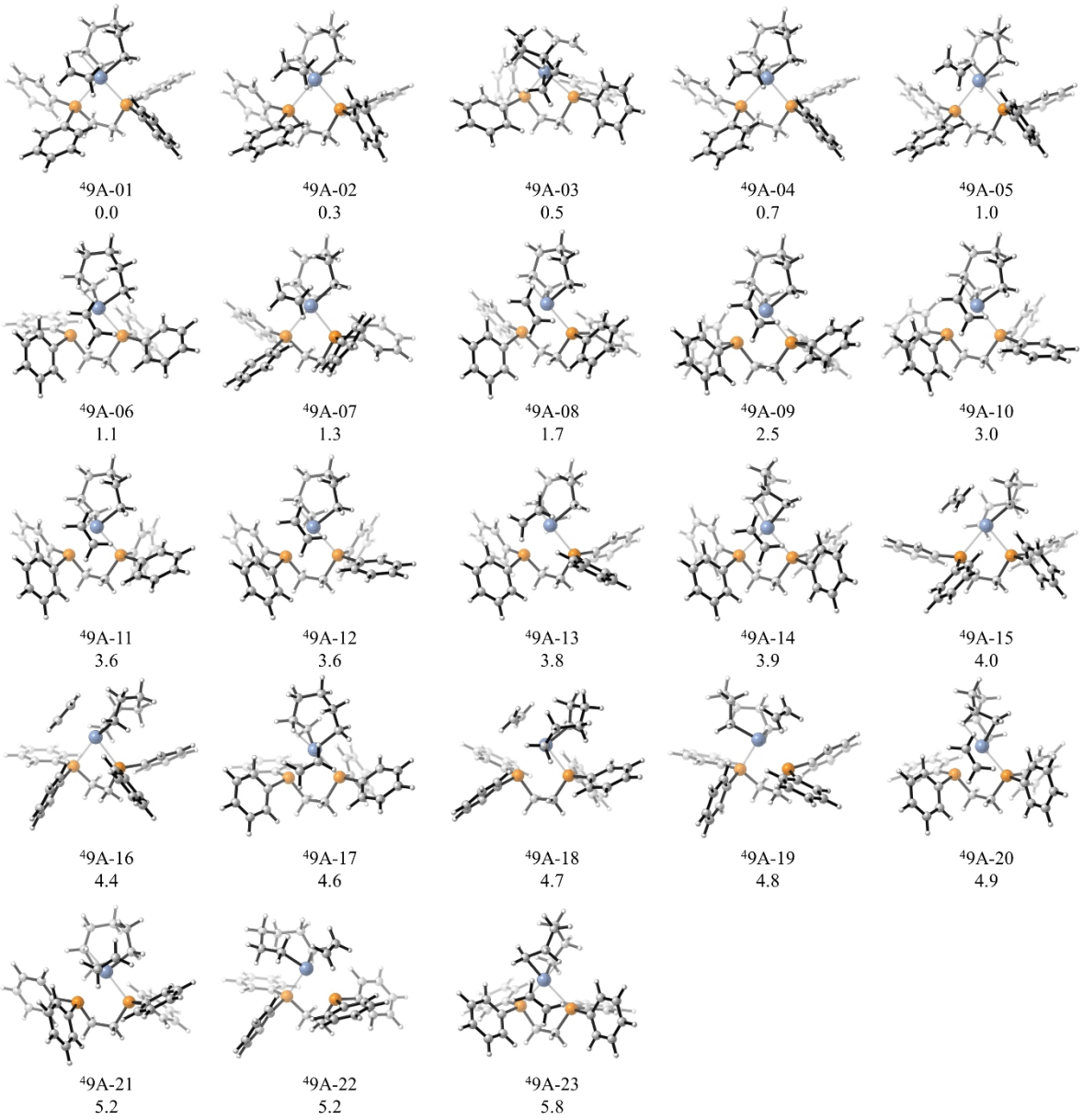

Fig. S14. Graphical representations of the conformers of [4]9 of catalyst model A. The Gibbs free energies (kcal/mol) relative to the lowest [4]9A are also shown.

Table S14. Relative Gibbs free energies for various conformers of ^{4}9B.

conformer	G (Hartree)	ΔG (kcal/mol)
1	-3273.863022	0.0
2	-3273.861419	1.0
3	-3273.861132	1.2
4	-3273.860830	1.4
5	-3273.860630	1.5
6	-3273.860438	1.6
7	-3273.859915	1.9
8	-3273.859796	2.0
9	-3273.859636	2.1
10	-3273.858818	2.6
11	-3273.858390	2.9
12	-3273.857032	3.8
13	-3273.856947	3.8
14	-3273.856620	4.0
15	-3273.856511	4.1
16	-3273.854714	5.2
17	-3273.852404	6.7
18	-3273.851829	7.0

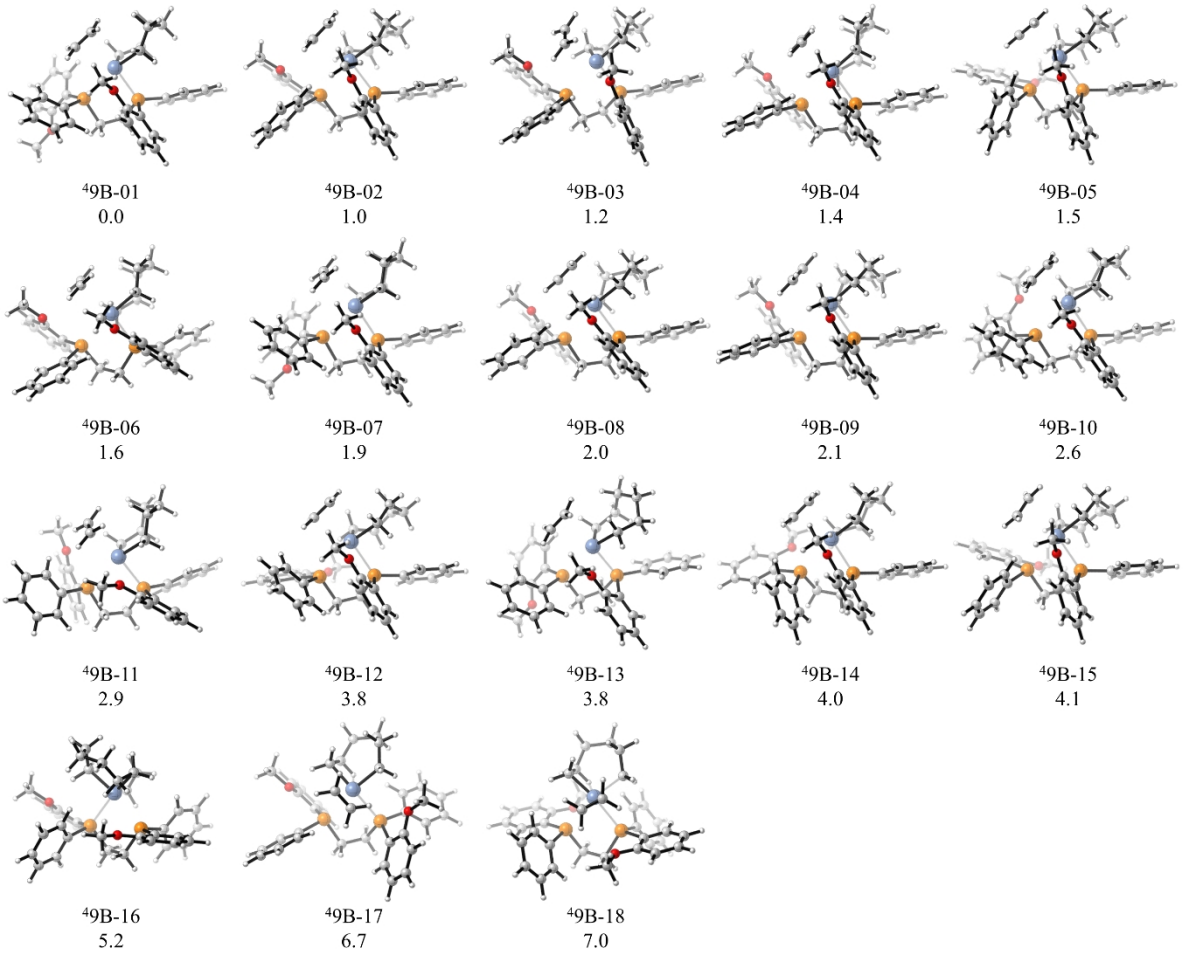

Fig. S15. Graphical representations of the conformers of [4]9 of catalyst model B. The Gibbs free energies (kcal/mol) relative to the lowest [4]9B are also shown.

8. Geometrical features of the intermediates and the transition states of catalyst model A and catalyst model B

Table S15. Geometrical features of the intermediates and the transition states of catalyst model A.

Intermediates	P-Cr-P angle (deg)	Cr-P distance (Å)	ΔCr-P (Å)
^{6}1A	82.4	2.551, 2.557	0.006
^{6}2A	82.9	2.549, 2.546	0.003
^{4}TS2-3A	76.9	2.469, 2.469	0
^{4}3A	82.9	2.597, 2.466	0.131
^{4}4A	79.8	2.589, 2.475	0.114
^{4}TS4-5A	79.4	2.493, 2.588	0.095
^{4}5A	81.4	2.459, 2.582	0.123
^{4}TS5-6A	78.9	2.499, 2.486	0.013
^{6}6A	83.4	2.559, 2.544	0.015
^{4}9A	80.9	2.469, 2.606	0.138
^{4}TS9-10A	78.1	2.514, 2.662	0.147
^{4}10A	80.4	2.641, 2.445	0.196
^{4}10A’	81.0	2.502, 2.477	0.025
^{4}TS10-11A	77.7	2.485, 2.509	0.024
^{6}11A	82.9	2.566, 2.561	0.005

Table S16. Geometrical features of the intermediates and the transition states of catalyst model B.

Intermediates	P-Cr-P angle (deg)	Cr-P distance (Å)	ΔCr-P (Å)	Cr-O distance (Å)	ΔCr-O (Å)
^{6}1B	82.3	2.540, 2.530	0.010	2.949, 2.777	0.172
^{6}2B	82.3	2.530, 2.535	0.006	3.211, 3.231	0.020
^{4}TS2-3B	76.0	2.482, 2.482	0	2.565, 2.565	0
^{4}3B	78.1	2.515, 2.533	0.018	2.166, 2.161	0.004
^{4}4B	78.8	2.421, 2.658	0.237	2.353, 4.014	1.661
^{4}TS4-5B	78.7	2.494, 2.552	0.059	2.396, 5.503	3.107
^{4}5B	80.6	2.481, 2.538	0.057	2.331, 5.419	3.087
^{4}TS5-6B	77.3	2.508, 2.463	0.045	2.613, 2.782	0.169
^{6}6B	82.9	2.538, 2.532	0.006	2.963,2.768	0.195
^{4}9B	78.3	2.437, 2.746	0.309	2.430, 5.720	3.290
^{4}TS9-10B	78.6	2.566, 2.501	0.065	2.416, 5.511	3.094
^{4}10B	81.0	2.399, 2.668	0.269	2.390, 3.997	1.607
^{4}10B’	83.2	2.500, 2.545	0.045	2.479, 3.551	1.071
^{4}TS10-11B	76.5	2.495, 2.552	0.058	2.542, 2.972	0.430
^{6}11B	82.5	2.544, 2.542	0.002	2.856, 2.987	0.131

9. Steric map for the intermediate 3 and 5

The topographic steric maps of the intermediates 3 and 5 were probed using SambVca. The center of the sphere is set to the location of atom Cr. C-C (from carbon bridge) defines the z-axis. P defines the xz-plane. The sphere radius is set to 3.5 Å.

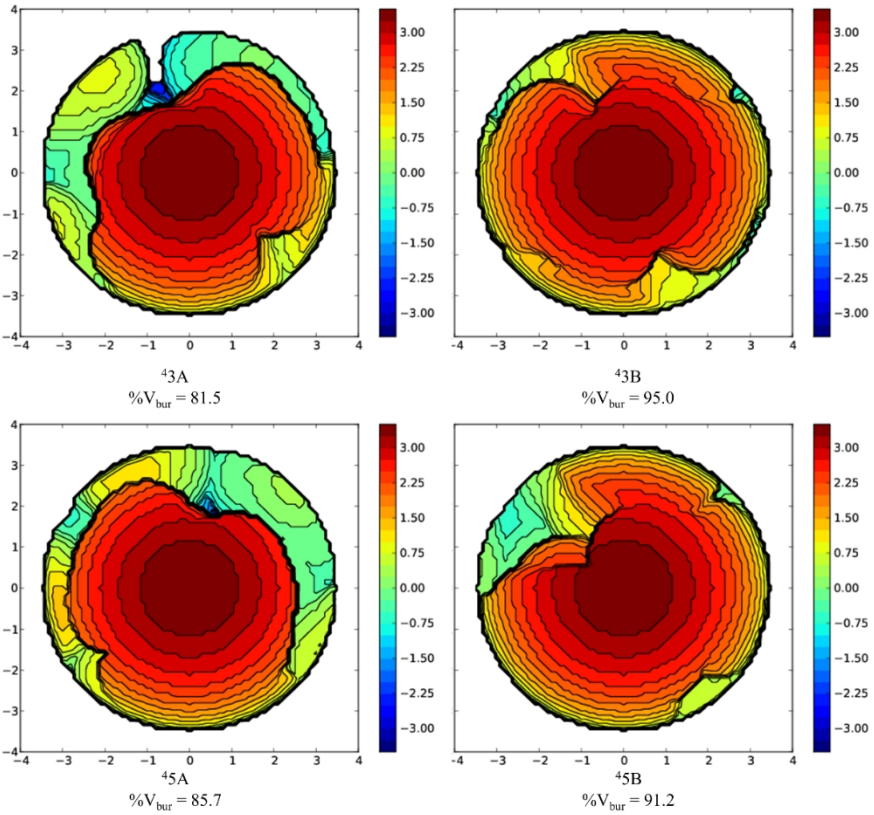

Fig. S16. Topographic steric maps of intermediate 3 (Top) and intermediate 5 (Bottom) of catalyst model A (Left) and catalyst model B (Right). The chromium center was removed for the buried volume calculations.

10. Graphical representations for the intermediates and transition states

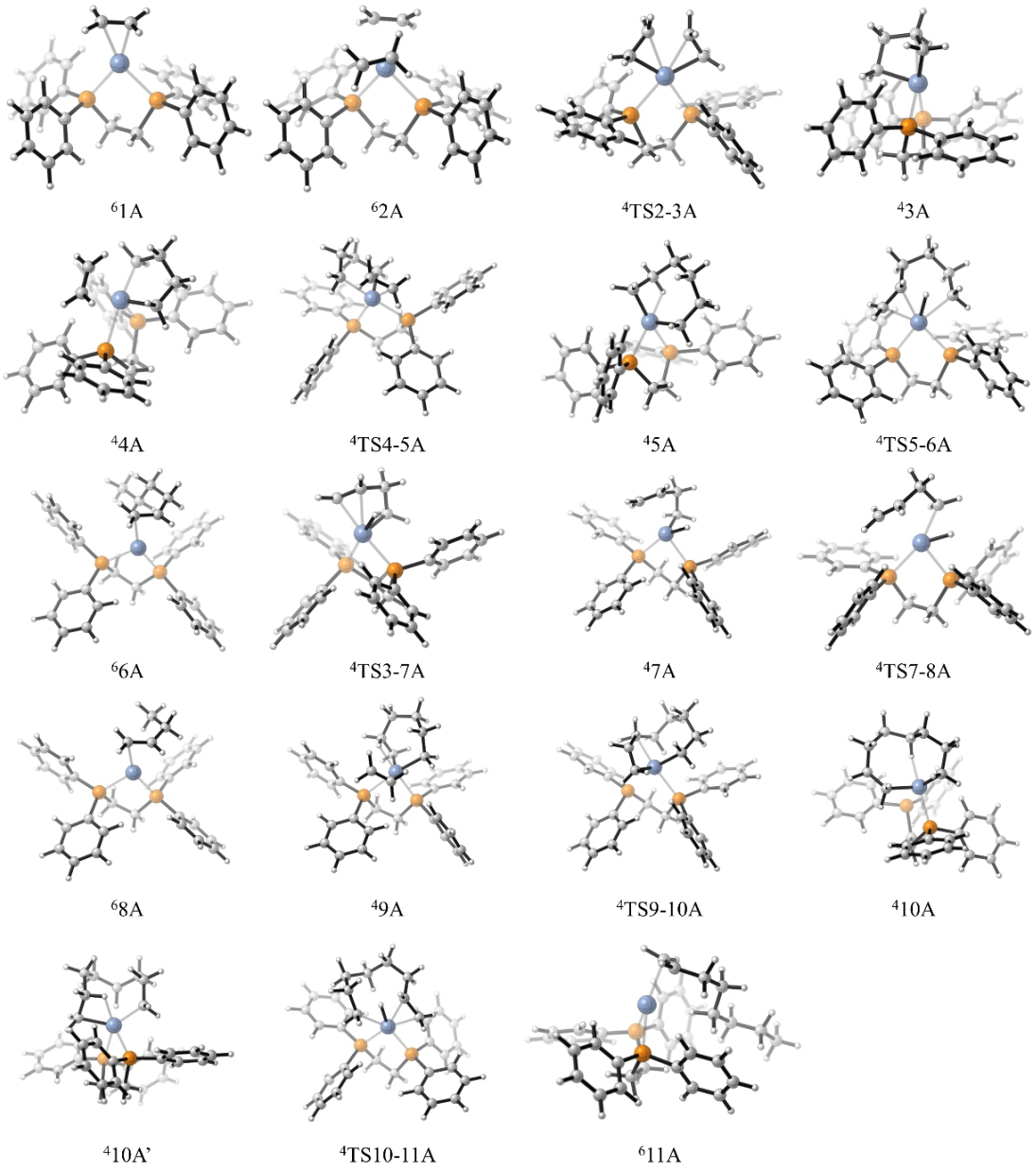

Fig. S17. Graphical representations for the intermediates and transition states of catalyst model A.

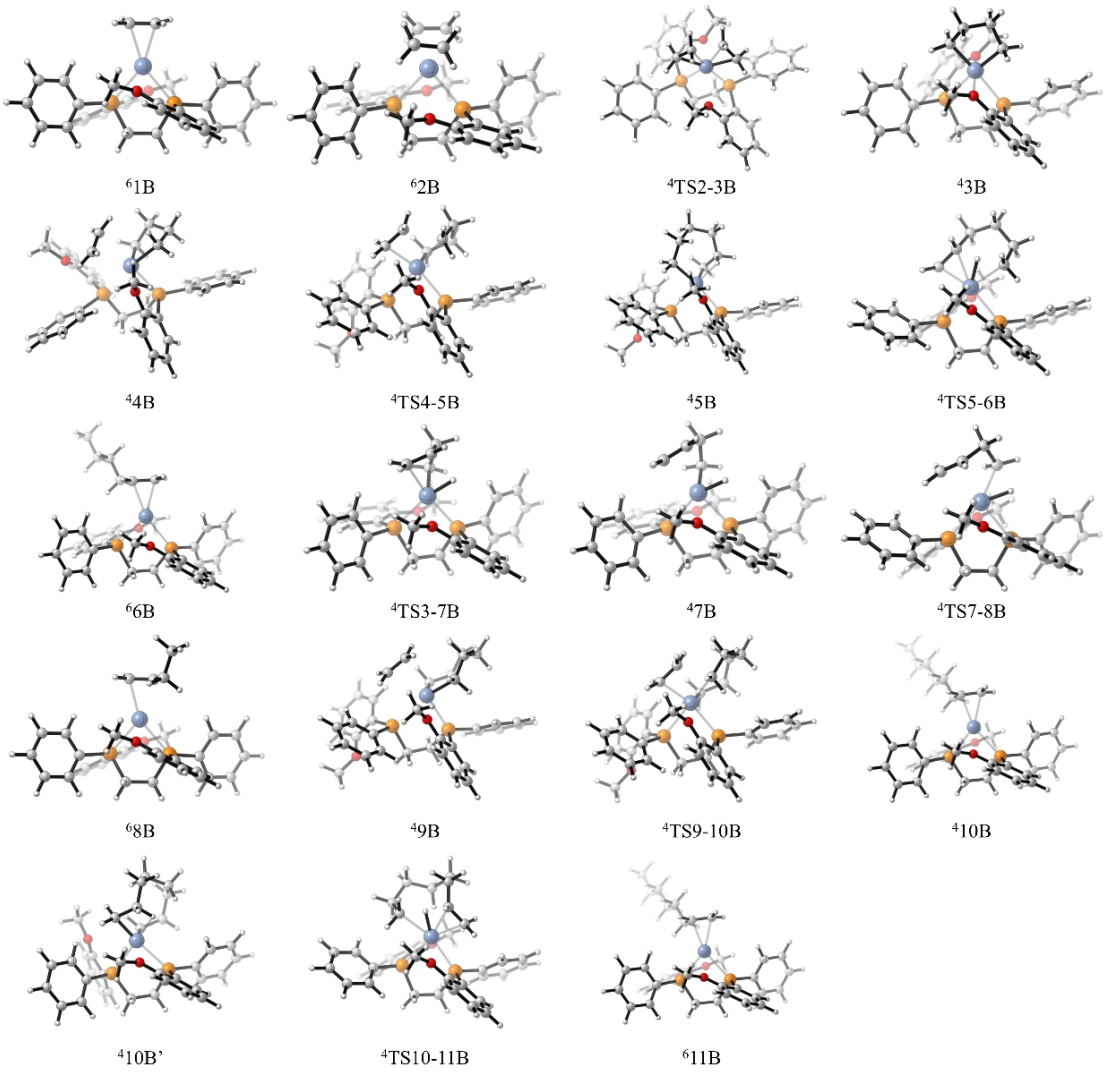

Fig. S18. Graphical representations for the intermediates and transition states of catalyst model B.

11. The Cr-PCCP^{Et} catalyst model C

CREST was utilized to generate an ensemble of conformers for the key intermediate 5, 9 and the key transition states TS5-6, TS9-10 of catalyst model C (Cr-PCCP^{Et}), respectively. The initial conformers were fully optimized at the B3LYP/def2-SVP level. The optimized geometries of the lowest energy conformation for the key intermediates and transition states are depicted in Fig. S11.

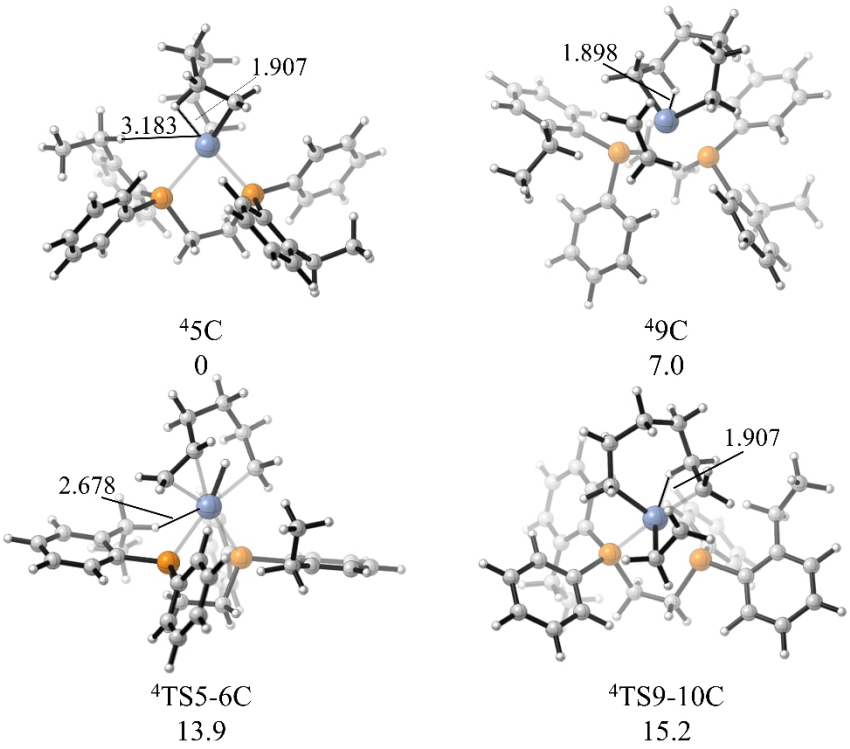

Fig. S19. Optimized geometries for the key intermediates and transition states of catalyst model C (Cr-PCCP^{Et}). Energy barriers in kcal/mol. Bond distances are in Å.

12. List of Cartesian Coordinates

^{6}1A
Geometry with 59 atoms:
Total energy: -2810.724594940

Cr	0.012420	-0.263240	1.768742
P	1.701873	0.036309	-0.126439
P	-1.661915	-0.041614	-0.142464
C	-0.650569	0.426412	-1.637740
C	0.715380	-0.273303	-1.683353
H	-1.224510	0.235758	-2.558315
H	-0.525653	1.519303	-1.572204
H	0.598563	-1.366195	-1.768166
H	1.286890	0.073728	-2.558409
C	3.175774	-1.038424	-0.257112
C	3.624368	-1.598049	-1.465844
C	3.889421	-1.298744	0.926751
C	4.767469	-2.403237	-1.484783
H	3.093156	-1.410680	-2.401119
C	5.035816	-2.095004	0.901736
H	3.546455	-0.873244	1.874615
C	5.475122	-2.650525	-0.304733
H	5.107635	-2.836623	-2.428482
H	5.584482	-2.287531	1.826942
H	6.368728	-3.279106	-0.324345
C	2.310885	1.757034	-0.359059
C	3.528817	2.046305	-0.996462
C	1.504796	2.816765	0.094853
C	3.925122	3.373599	-1.182229
H	4.173829	1.236216	-1.344723
C	1.900016	4.142484	-0.101002
H	0.559185	2.610378	0.605136
C	3.112341	4.422213	-0.739203
H	4.875849	3.589374	-1.676065
H	1.263639	4.957648	0.252121
H	3.426725	5.458307	-0.886521
C	-2.412579	-1.670849	-0.539609
C	-3.173970	-2.287475	0.471431
C	-2.242865	-2.332041	-1.766522
C	-3.764707	-3.532532	0.253218
H	-3.316533	-1.783541	1.432378
C	-2.828473	-3.585342	-1.977952
H	-1.657190	-1.879825	-2.569042
C	-3.589892	-4.185976	-0.972410
H	-4.361640	-3.996580	1.042174
H	-2.689654	-4.091303	-2.936553
H	-4.047389	-5.163741	-1.141690
C	-3.049770	1.153534	-0.170934
C	-4.070282	1.074573	-1.134140
C	-3.072366	2.188140	0.778762
C	-5.090767	2.027429	-1.150434
H	-4.073549	0.262254	-1.865715
C	-4.094320	3.141996	0.757356
H	-2.293384	2.245174	1.545346
C	-5.102574	3.062185	-0.207552
H	-5.883112	1.961228	-1.900163
H	-4.107210	3.943776	1.499753
H	-5.904714	3.804241	-0.222038
C	0.708313	-0.797465	3.927243
C	-0.662448	-0.767996	3.944918
H	1.254983	-1.736311	3.782002
H	1.301497	0.069745	4.239658
H	-1.210587	0.123162	4.271627
H	-1.252291	-1.682519	3.814317

^{6}2A
Geometry with 65 atoms:
Total energy: -2889.321313180

Cr	0.009004	-0.215780	1.620061
P	1.699212	0.055824	-0.264569
P	-1.673829	-0.031764	-0.285742
C	-0.652796	0.416093	-1.782615
C	0.709454	-0.290584	-1.812111
H	-1.225171	0.217823	-2.702520
H	-0.523279	1.508993	-1.729322
H	0.583917	-1.384411	-1.864569
H	1.281702	0.025548	-2.698481
C	3.161296	-1.039755	-0.368103
C	3.541166	-1.728503	-1.532262
C	3.935951	-1.184639	0.797890
C	4.674956	-2.547775	-1.525593
H	2.964937	-1.630600	-2.454177
C	5.072762	-1.994859	0.797530
H	3.648926	-0.654575	1.711025
C	5.441927	-2.681071	-0.364746
H	4.961703	-3.080823	-2.435496
H	5.669059	-2.095492	1.707660
H	6.327765	-3.320852	-0.364574
C	2.346270	1.754359	-0.561915
C	3.572038	1.996199	-1.204246
C	1.562400	2.846608	-0.149468
C	3.997944	3.307702	-1.433016
H	4.200335	1.161246	-1.523112
C	1.985754	4.156380	-0.389055
H	0.612812	2.674076	0.364144
C	3.206752	4.388413	-1.029736
H	4.955064	3.485926	-1.929571
H	1.365099	4.996472	-0.067547
H	3.544483	5.411889	-1.209991
C	-2.481414	-1.629512	-0.691859
C	-3.305991	-2.202826	0.295369
C	-2.281899	-2.319896	-1.897885
C	-3.927628	-3.432029	0.074003
H	-3.468839	-1.678518	1.241891
C	-2.896617	-3.559203	-2.111419
H	-1.649878	-1.901892	-2.683577
C	-3.720376	-4.115753	-1.130235
H	-4.573162	-3.861072	0.844312
H	-2.732630	-4.087547	-3.053874
H	-4.201479	-5.081757	-1.301575
C	-3.023294	1.212308	-0.312140
C	-4.222744	1.016529	-1.016545
C	-2.824264	2.415689	0.387364
C	-5.202124	2.013661	-1.022165
H	-4.397636	0.083424	-1.557305
C	-3.801375	3.414026	0.371415
H	-1.899498	2.575019	0.950087
C	-4.993352	3.212218	-0.331963
H	-6.134039	1.852620	-1.569807
H	-3.635938	4.346882	0.916050
H	-5.762662	3.988310	-0.338362
C	-0.419349	-2.541339	2.484462
C	0.857209	-2.230567	2.812926
H	-1.246025	-2.389974	3.186567
H	-0.665177	-3.051308	1.547112
H	1.696575	-2.488902	2.158387
H	1.112112	-1.826922	3.798744
C	-0.846472	0.975731	3.577033
C	0.439192	1.393143	3.433951
H	-1.682930	1.528433	3.136260
H	-1.107314	0.153705	4.251835
H	1.259592	0.920789	3.984357
H	0.692474	2.296818	2.869452

^{4}TS2-3A
Geometry with 65 atoms:
Total energy: -2889.281639100

Cr	-0.000046	-0.000163	1.547121
P	-1.535223	0.060268	-0.386233
P	1.535253	-0.060163	-0.386147
C	0.682812	0.343768	-1.996147
C	-0.682677	-0.343283	-1.996272
H	0.570673	1.437684	-2.056736
H	1.307489	0.025835	-2.844772
H	-1.307298	-0.025149	-2.844863
H	-0.570535	-1.437184	-2.057111
C	-2.026177	1.808381	-0.640750
C	-1.479281	2.797119	0.193144
C	-2.874754	2.188974	-1.694995
C	-1.767914	4.147588	-0.023585
H	-0.827371	2.507626	1.024491
C	-3.167907	3.537874	-1.905851
H	-3.314815	1.430534	-2.347657
C	-2.613428	4.517541	-1.073252
H	-1.336858	4.908934	0.630879
H	-3.831871	3.827008	-2.724061
H	-2.844302	5.572093	-1.242762
C	-3.058013	-0.948612	-0.371086
C	-4.300287	-0.401728	-0.008545
C	-2.958302	-2.330684	-0.616682
C	-5.427314	-1.223032	0.087029
H	-4.394044	0.666574	0.196399
C	-4.088630	-3.145135	-0.521594
H	-1.998035	-2.782677	-0.880678
C	-5.325290	-2.592997	-0.170786
H	-6.390169	-0.787087	0.364322
H	-4.002796	-4.215998	-0.721729
H	-6.208652	-3.231873	-0.097046
C	3.058059	0.948688	-0.370675
C	2.958387	2.330818	-0.615960
C	4.300302	0.401700	-0.008184
C	4.088725	3.145227	-0.520619
H	1.998144	2.782890	-0.879908
C	5.427338	1.222961	0.087645
H	4.394027	-0.666651	0.196523
C	5.325354	2.592986	-0.169865
H	4.002922	4.216137	-0.720515
H	6.390168	0.786936	0.364896
H	6.208723	3.231830	-0.095927
C	2.026196	-1.808224	-0.641038
C	2.874835	-2.188584	-1.695318
C	1.479229	-2.797150	0.192587
C	3.167979	-3.537439	-1.906472
H	3.314950	-1.429998	-2.347773
C	1.767854	-4.147573	-0.024440
H	0.827268	-2.507844	1.023960
C	2.613430	-4.517293	-1.074139
H	3.831992	-3.826392	-2.724707
H	1.336743	-4.909065	0.629817
H	2.844298	-5.571809	-1.243883
C	-1.830371	0.108382	2.533267
C	-0.937058	0.298048	3.661518
H	-2.434463	0.969090	2.222886
H	-2.388677	-0.836383	2.494914
H	-1.111240	-0.345755	4.529376
H	-0.800920	1.343020	3.968152
C	1.830214	-0.108952	2.533359
C	0.936830	-0.298874	3.661509
H	2.434317	-0.969594	2.222814
H	2.388531	0.835816	2.495260
H	1.110958	0.344730	4.529525
H	0.800668	-1.343916	3.967895

^{4}3A
Geometry with 65 atoms:
Total energy: -2889.288474050

Cr	0.104363	-0.120013	1.548277
P	1.639195	0.162768	-0.361073
P	-1.711555	0.064813	-0.299095
C	-0.753012	0.618309	-1.798313
C	0.617713	-0.064483	-1.905775
H	-1.346596	0.461045	-2.712540
H	-0.639417	1.708486	-1.686817
H	0.507272	-1.152507	-2.041796
H	1.173276	0.328640	-2.771347
C	3.052585	-0.976630	-0.531779
C	3.466956	-1.481819	-1.776655
C	3.754710	-1.339777	0.630903
C	4.567329	-2.340348	-1.851470
H	2.945133	-1.210287	-2.696247
C	4.856090	-2.193821	0.548450
H	3.435523	-0.953930	1.600953
C	5.262282	-2.696808	-0.691945
H	4.882636	-2.730819	-2.822058
H	5.395702	-2.471691	1.456971
H	6.120752	-3.369926	-0.754755
C	2.308677	1.865356	-0.481994
C	3.590506	2.132685	-0.989110
C	1.504392	2.932866	-0.042398
C	4.052888	3.449680	-1.061547
H	4.233391	1.314694	-1.320935
C	1.968053	4.247630	-0.122896
H	0.506904	2.745613	0.366203
C	3.244816	4.506856	-0.631720
H	5.053180	3.649311	-1.453355
H	1.335187	5.069755	0.219819
H	3.612691	5.534192	-0.687218
C	-2.503156	-1.522086	-0.753845
C	-3.284549	-2.157435	0.229402

C -2.338213 -2.139858 -2.003287
C -3.903750 -3.377957 -0.040876
H -3.416823 -1.691808 1.210659
C -2.954221 -3.368253 -2.267178
H -1.733953 -1.673558 -2.783650
C -3.738130 -3.986856 -1.290577
H -4.515359 -3.858003 0.726820
H -2.821279 -3.839873 -3.243889
H -4.220007 -4.944683 -1.500845
C -3.075402 1.280591 -0.177165
C -4.141344 1.288400 -1.093829
C -3.031981 2.248887 0.839866
C -5.139106 2.260269 -0.997279
H -4.196674 0.528765 -1.878066
C -4.032008 3.221584 0.932413
H -2.219467 2.246455 1.572932
C -5.084475 3.228124 0.012899
H -5.965933 2.261842 -1.711755
H -3.992103 3.969859 1.727783
H -5.868823 3.985521 0.086232
C 0.186190 -2.150580 1.762841
C -0.021820 -2.150053 3.287337
H -0.620292 -2.634448 1.191382
H 1.162953 -2.536491 1.435915
H 0.794803 -2.683511 3.802037
H -0.965978 -2.642004 3.571422
C -0.021873 -0.680998 3.781647
C 1.199819 0.054141 3.252688
H -0.960107 -0.183829 3.366154
H -0.204660 -0.583964 4.865768
H 2.135287 -0.509350 3.374572
H 1.313658 1.087424 3.620673

^{4}4A
Geometry with 71 atoms:
Total energy: -2967.891944300
Cr 0.043880 -0.629295 1.340029
P -1.741297 -0.013571 -0.430789
P 1.505255 0.128793 -0.507628
C 0.481748 0.528279 -2.023657
C -0.847567 -0.235358 -2.048609
H 0.298908 1.613492 -1.988361
H 1.070658 0.326210 -2.930889
H -1.484743 0.109577 -2.878153
H -0.676344 -1.314320 -2.182423
C -2.188752 1.766707 -0.441341
C -1.388894 2.657646 0.296077
C -3.258285 2.275376 -1.199458
C -1.646868 4.031045 0.275774
H -0.543090 2.287681 0.882386
C -3.520540 3.647222 -1.210367
H -3.892894 1.598934 -1.777287
C -2.716767 4.526179 -0.474681
H -1.011285 4.710814 0.848287
H -4.356856 4.033542 -1.798050
H -2.926190 5.598574 -0.486957
C -3.310653 -0.938062 -0.583699
C -4.412009 -0.558636 0.207802
C -3.418376 -2.077269 -1.400542
C -5.595573 -1.298014 0.174152
H -4.352911 0.329118 0.841521
C -4.606259 -2.814040 -1.429455
H -2.584795 -2.402227 -2.025482
C -5.695653 -2.428251 -0.644171
H -6.445006 -0.986804 0.787068
H -4.678602 -3.693274 -2.074140
H -6.623117 -3.005127 -0.671317
C 2.394217 1.681436 -0.118779
C 3.021542 2.424191 -1.134927
C 2.437541 2.148946 1.205128
C 3.672511 3.620175 -0.827871
H 3.006989 2.067722 -2.168073
C 3.091387 3.347480 1.508471
H 1.977325 1.569704 2.009820
C 3.706718 4.083761 0.492836
H 4.158692 4.192210 -1.621743
H 3.124403 3.701244 2.541682
H 4.219923 5.018948 0.729872
C 2.779171 -1.056011 -1.067288
C 2.447597 -2.071938 -1.980301
C 4.069226 -1.019520 -0.512684
C 3.395424 -3.033910 -2.335380
H 1.448075 -2.126228 -2.416968
C 5.012476 -1.986349 -0.870081
H 4.343026 -0.231988 0.192498
C 4.678023 -2.994937 -1.778757
H 3.129620 -3.818469 -3.047781
H 6.015025 -1.948338 -0.437416
H 5.417587 -3.749878 -2.055832
C -0.018114 -2.605333 0.779210
C 1.236412 -3.290712 1.315815
H -0.929574 -2.910904 1.331986
H -0.193374 -2.780907 -0.295832
H 2.069483 -3.136469 0.610049
H 1.097087 -4.386380 1.391487
C 1.610913 -2.678679 2.672357
C 1.695842 -1.150628 2.535352
H 0.839203 -2.955560 3.415510
H 2.555738 -3.114501 3.048991
H 2.616364 -0.882535 1.986333
H 1.758796 -0.642980 3.514542
C -1.018084 -0.499916 3.694115
C -2.041868 -0.339881 2.831596
H -0.723878 -1.487164 4.059905
H -0.494073 0.357726 4.127703
H -2.395261 0.657062 2.547245
H -2.626313 -1.189741 2.465564

^{4}TS4-5A
Geometry with 71 atoms:
Total energy: -2967.875960250
Cr -0.121560 -0.684314 1.298105
P -1.720681 0.084510 -0.452658
P 1.523499 0.189673 -0.498546
C 0.518844 0.679578 -2.000627
C -0.820809 -0.064326 -2.074343
H 0.352421 1.764301 -1.910418
H 1.111227 0.519073 -2.913745
H -1.448016 0.329615 -2.889409
H -0.660110 -1.137499 -2.260226
C -2.178948 1.858490 -0.380910
C -1.358434 2.735134 0.349782
C -3.282806 2.375242 -1.081672
C -1.627973 4.106127 0.374044
H -0.490123 2.355935 0.894677
C -3.554995 3.744737 -1.048078
H -3.936136 1.707805 -1.648796
C -2.728666 4.611524 -0.323480
H -0.976693 4.776801 0.939606
H -4.416974 4.138105 -1.592472
H -2.945130 5.682374 -0.302210
C -3.282071 -0.846118 -0.626824
C -4.327114 -0.575063 0.277238
C -3.437284 -1.882917 -1.562115
C -5.505891 -1.320885 0.237357
H -4.223582 0.228590 1.010011
C -4.619958 -2.628681 -1.595034
H -2.645137 -2.121651 -2.273559
C -5.654649 -2.350673 -0.698384
H -6.311998 -1.096317 0.939968
H -4.730852 -3.430394 -2.329230
H -6.577610 -2.934705 -0.728024
C 2.467182 1.698016 -0.063328
C 3.268778 2.354281 -1.014667
C 2.373430 2.222311 1.236176
C 3.952806 3.520911 -0.669904
H 3.363717 1.949182 -2.025473
C 3.061589 3.390626 1.579896
H 1.768240 1.716805 1.994626
C 3.848720 4.041015 0.626193
H 4.573609 4.025572 -1.414170
H 2.984891 3.789100 2.594358
H 4.387888 4.953351 0.892756
C 2.775989 -0.999877 -1.102091
C 2.481608 -1.897135 -2.142850
C 4.002626 -1.113040 -0.423579
C 3.400727 -2.887758 -2.499053
H 1.533883 -1.838005 -2.682440
C 4.917478 -2.104637 -0.784393
H 4.249242 -0.421976 0.386278
C 4.617864 -2.995891 -1.819880
H 3.162800 -3.578409 -3.311671
H 5.869709 -2.180426 -0.253817
H 5.333696 -3.772611 -2.098986
C -0.116612 -2.610495 0.586440
C 1.144726 -3.305575 1.087239
H -1.033659 -3.029809 1.039982
H -0.223189 -2.660959 -0.510491
H 2.011416 -2.976557 0.491547
H 1.080903 -4.401004 0.945637
C 1.398985 -2.977206 2.562697
C 1.306332 -1.479558 2.832620
H 0.665196 -3.509630 3.195058
H 2.390812 -3.355038 2.873526
H 1.993003 -0.908248 2.173487
H 1.595271 -1.216978 3.856375
C -0.708973 -0.992327 3.586588
C -1.731527 -0.617750 2.693438
H -0.688287 -2.007441 3.989583
H -0.301597 -0.233085 4.260374
H -2.088073 0.419542 2.706998
H -2.461411 -1.363096 2.362853

^{4}5A
Geometry with 71 atoms:
Total energy: -2967.916449150
Cr -0.065208 -0.811324 1.083741
C 0.073744 -2.583737 0.059921
C 1.074234 -3.588694 0.630366
H 1.128195 -4.446253 -0.067174
H 2.094188 -3.160255 0.633227
C 0.725898 -4.129766 2.026633
H 1.232970 -5.096524 2.179719
C 1.116135 -3.219711 3.200165
C 0.616479 -1.770542 3.123051
C -0.841177 -1.538343 2.808725
H -1.319143 -0.762597 3.428221
H -1.464209 -2.440183 2.763620
H 0.956563 -1.202124 4.004664
H 1.293560 -1.268691 2.316647
H 0.733697 -3.654201 4.139197
H 2.216126 -3.202325 3.292249
H -0.354745 -4.353052 2.062918
H 0.339058 -2.319777 -0.978511
H -0.945671 -3.007063 0.049922
P -1.759303 0.093501 -0.451672
C -3.348990 -0.738942 -0.783437
C -4.211271 -0.281173 -1.794945
C -5.425934 -0.929585 -2.021901
C -5.789377 -2.032607 -1.239557
C -4.938696 -2.485312 -0.227485
C -3.719654 -1.840766 0.003658
H -3.056884 -2.190540 0.798212
H -5.223549 -3.343147 0.386369
H -6.741657 -2.537704 -1.419176
H -6.094227 -0.571517 -2.808724
H -3.941424 0.587522 -2.401173
C -2.138330 1.825370 0.025347
C -2.268010 2.870787 -0.904464
C -2.518656 4.173956 -0.466566
C -2.648172 4.445697 0.899298
C -2.531957 3.409644 1.831340
C -2.276116 2.106368 1.397635
H -2.191541 1.299443 2.132152
H -2.640585 3.615955 2.898872
H -2.842264 5.466621 1.236883
H -2.612996 4.981316 -1.196825
H -2.169657 2.679973 -1.975284
C -0.889167 0.207595 -2.091494
C 0.443518 0.964186 -1.988260
P 1.509701 0.431903 -0.541905
C 2.800716 -0.690754 -1.185369
C 2.665606 -1.365246 -2.408880
C 3.615327 -2.316089 -2.797398
C 4.705653 -2.600383 -1.971881
C 4.844712 -1.934235 -0.748587
C 3.894410 -0.992636 -0.351838
H 4.007962 -0.484964 0.610141
H 5.695038 -2.153082 -0.098158
H 5.446646 -3.342129 -2.279053
H 3.499327 -2.835527 -3.751640
H 1.817969 -1.164926 -3.067382
C 2.337949 1.981818 -0.028734

C	1.643358	2.811427	0.870664
C	2.186664	4.037015	1.261529
C	3.432052	4.438371	0.766775
C	4.128250	3.615807	-0.125075
C	3.584753	2.392575	-0.527660
H	4.133999	1.759493	-1.228071
H	5.099867	3.929566	-0.514552
H	3.861452	5.394103	1.077085
H	1.637358	4.677087	1.956173
H	0.665315	2.509312	1.257772
H	0.259531	2.034435	-1.812323
H	1.015235	0.896229	-2.926703
H	-0.746263	-0.835954	-2.413930
H	-1.543896	0.679633	-2.840948

^{4}TS5-6A
Geometry with 71 atoms:
Total energy: -2967.891857410

Cr	-0.016021	-0.057269	1.290493
P	-1.581017	0.425961	-0.596658
P	1.584785	0.411283	-0.553085
C	0.721910	0.654805	-2.199299
C	-0.690438	1.222273	-2.031610
H	1.337229	1.289530	-2.855572
H	0.684401	-0.341552	-2.664696
H	-0.666189	2.298263	-1.794279
H	-1.275458	1.104009	-2.956378
C	-3.012275	1.526511	-0.303672
C	-3.795248	2.010939	-1.368564
C	-3.317184	1.923306	1.009029
C	-4.865637	2.871843	-1.118134
H	-3.578061	1.713216	-2.397102
C	-4.390540	2.784447	1.255264
H	-2.716653	1.556878	1.844425
C	-5.165586	3.257898	0.193334
H	-5.469219	3.242313	-1.950275
H	-4.619689	3.085704	2.280203
H	-6.004539	3.931029	0.386112
C	-2.240740	-1.160431	-1.256630
C	-3.615173	-1.403662	-1.411161
C	-1.327437	-2.195854	-1.540088
C	-4.063868	-2.650020	-1.860843
H	-4.343758	-0.625606	-1.177685
C	-1.780740	-3.435213	-1.995740
H	-0.253318	-2.049901	-1.400552
C	-3.151186	-3.665080	-2.157895
H	-5.136167	-2.826141	-1.976271
H	-1.060183	-4.226319	-2.217178
H	-3.506319	-4.637044	-2.508627
C	2.594452	1.923332	-0.316557
C	3.803180	1.856682	0.399730
C	2.132057	3.172678	-0.765756
C	4.537915	3.017758	0.649496
H	4.180355	0.895066	0.753530
C	2.869656	4.331980	-0.508798
H	1.195724	3.255515	-1.322199
C	4.073057	4.257427	0.198148
H	5.480604	2.952160	1.198189
H	2.501829	5.296476	-0.867162
H	4.649687	5.164289	0.395557
C	2.767584	-0.942832	-0.906283
C	3.849258	-0.756200	-1.784467
C	2.540664	-2.214086	-0.353182
C	4.685728	-1.828331	-2.102465
H	4.044623	0.229234	-2.214331
C	3.378097	-3.285910	-0.675941
H	1.709483	-2.372536	0.339184
C	4.451084	-3.093058	-1.550628
H	5.526028	-1.675920	-2.784122
H	3.194724	-4.270180	-0.238440
H	5.108804	-3.928803	-1.801488
C	1.748542	0.071035	2.455119
C	0.746922	-0.491219	3.327157
C	0.795064	-1.983170	3.678483
C	-0.588115	-2.612879	3.899198
C	-1.508425	-2.503149	2.672749
C	-1.843911	-1.054330	2.284151
H	2.573458	-0.574036	2.130687
H	2.040046	1.118423	2.597491
H	0.423808	0.144428	4.167784
H	-0.539999	-0.490182	2.794174
H	1.315158	-2.525523	2.867874
H	1.419847	-2.112361	4.578750
H	-1.078467	-2.125208	4.761941
H	-0.462194	-3.672292	4.175270
H	-1.036084	-3.021649	1.815984
H	-2.445154	-3.055543	2.867894
H	-2.543661	-1.029911	1.440016
H	-2.354716	-0.544963	3.120750

^{6}6A
Geometry with 71 atoms:
Total energy: -2967.966560500

Cr	-0.005632	-0.191213	1.534957
P	1.681732	0.671243	-0.161942
P	-1.701627	0.431750	-0.277318
C	-0.675344	1.240156	-1.610031
C	0.719348	0.616091	-1.764599
H	-1.221773	1.236321	-2.566463
H	-0.589916	2.295700	-1.303759
H	0.652560	-0.445025	-2.054628
H	1.282473	1.141388	-2.552060
C	3.142499	-0.394112	-0.459470
C	3.580794	-0.775836	-1.739095
C	3.829949	-0.872811	0.670749
C	4.683771	-1.623955	-1.880787
H	3.070359	-0.418395	-2.635438
C	4.937609	-1.710259	0.525281
H	3.490779	-0.590940	1.671995
C	5.363123	-2.091199	-0.752047
H	5.014013	-1.918468	-2.880019
H	5.465616	-2.072778	1.410647
H	6.223909	-2.754332	-0.867117
C	2.296488	2.400421	-0.108486
C	3.469905	2.803367	-0.767901
C	1.535430	3.354797	0.588820
C	3.867068	4.142387	-0.735018
H	4.079039	2.070702	-1.302898
C	1.931242	4.695095	0.611716
H	0.629750	3.051268	1.122313
C	3.098167	5.089583	-0.049660
H	4.782995	4.447876	-1.246973
H	1.331405	5.430663	1.153285
H	3.412968	6.135713	-0.026453
C	-2.477940	-1.043112	-1.045507
C	-3.378344	-1.776975	-0.249760
C	-2.157224	-1.518146	-2.326798
C	-3.948110	-2.957152	-0.727692
H	-3.640167	-1.417632	0.749938
C	-2.721178	-2.709665	-2.798217
H	-1.468882	-0.970086	-2.972818
C	-3.613726	-3.431171	-2.002177
H	-4.651777	-3.512233	-0.102459
H	-2.462034	-3.070861	-3.796495
H	-4.052569	-4.360232	-2.373713
C	-3.073227	1.619830	-0.017720
C	-4.129473	1.750694	-0.935492
C	-3.037620	2.446390	1.117351
C	-5.128131	2.702934	-0.720429
H	-4.176755	1.102779	-1.814532
C	-4.036295	3.401723	1.327058
H	-2.228927	2.338545	1.846689
C	-5.081743	3.530110	0.407838
H	-5.948627	2.799013	-1.435877
H	-4.002181	4.040263	2.213237
H	-5.866616	4.272320	0.573094
C	0.735197	-1.443912	3.352209
C	-0.563829	-1.850953	3.193107
C	-1.028642	-3.137510	2.546174
C	-0.022243	-3.913422	1.688781
C	0.290405	-3.277982	0.330670
C	1.293183	-4.073193	-0.501676
H	1.575763	-2.035005	2.975317
H	0.984448	-0.626930	4.038884
H	-1.344623	-1.303779	3.739327
H	2.265383	-4.155497	0.011766
H	-1.367607	-3.784354	3.378603
H	-1.941716	-2.940635	1.957516
H	-0.434811	-4.920871	1.510620
H	0.913255	-4.073579	2.253232
H	-0.649648	-3.150560	-0.232489
H	0.698454	-2.256626	0.475042
H	0.927863	-5.096093	-0.692210
H	1.474537	-3.596712	-1.478336

^{4}TS3-7A
Geometry with 65 atoms:
Total energy: -2889.263107110

Cr	0.039812	-0.673826	1.424935
P	1.668507	0.175882	-0.289661
P	-1.626191	0.037958	-0.276390
C	-0.663385	0.589137	-1.780964
C	0.717901	-0.076011	-1.872597
H	-1.251401	0.411311	-2.694175
H	-0.557489	1.680614	-1.681323
H	0.627975	-1.164856	-2.017375
H	1.287495	0.335246	-2.720699
C	3.251999	-0.710481	-0.477154
C	3.598287	-1.434788	-1.629447
C	4.136483	-0.690611	0.618063
C	4.812810	-2.127120	-1.682697
H	2.932508	-1.465419	-2.493909
C	5.350316	-1.375839	0.555505
H	3.877611	-0.130906	1.521365
C	5.688592	-2.098636	-0.594487
H	5.074890	-2.688811	-2.582600
H	6.033013	-1.349975	1.408287
H	6.636419	-2.640255	-0.640562
C	2.061695	1.966294	-0.293289
C	3.219741	2.476273	-0.904141
C	1.143403	2.854344	0.296009
C	3.448314	3.854257	-0.928538
H	3.946606	1.797900	-1.357128
C	1.372444	4.232245	0.261726
H	0.235852	2.477381	0.776917
C	2.525935	4.732879	-0.349734
H	4.351798	4.243992	-1.403829
H	0.649724	4.913890	0.716533
H	2.709185	5.809863	-0.372370
C	-2.696450	-1.341535	-0.826866
C	-3.728667	-1.757142	0.032914
C	-2.460781	-2.048912	-2.015591
C	-4.522100	-2.854571	-0.302796
H	-3.913646	-1.219167	0.966655
C	-3.255707	-3.152459	-2.344280
H	-1.657227	-1.753262	-2.693287
C	-4.285809	-3.555832	-1.491282
H	-5.327266	-3.166208	0.366985
H	-3.066633	-3.697206	-3.272455
H	-4.905121	-4.417911	-1.750464
C	-2.753413	1.431740	0.081537
C	-3.677562	1.876412	-0.880608
C	-2.671591	2.089450	1.319474
C	-4.497254	2.972412	-0.607709
H	-3.763686	1.360418	-1.840630
C	-3.495034	3.187402	1.588955
H	-1.974396	1.737844	2.085537
C	-4.404731	3.630152	0.625059
H	-5.214259	3.314270	-1.358034
H	-3.428298	3.693214	2.555108
H	-5.049189	4.487134	0.835600
C	0.137066	-2.641726	0.789405
C	-0.116040	-3.243385	2.180252
H	-0.626743	-2.909453	0.047162
H	1.141533	-2.853830	0.389136
H	0.557382	-4.089635	2.410622
H	-1.149770	-3.605165	2.274201
C	0.132796	-2.129776	3.196141
C	1.317103	-1.402350	3.087310
H	-1.141316	-1.118277	2.505464
H	-0.464449	-2.096105	4.112367
H	2.122138	-1.768272	2.441719
H	1.598360	-0.675061	3.856478

^{4}7A
Geometry with 65 atoms:
Total energy: -2889.271658410

Cr	0.001132	-0.672784	1.437132
P	1.616714	0.218628	-0.339001
P	-1.631862	0.002652	-0.260384
C	-0.731356	0.579612	-1.791456
C	0.655782	-0.066521	-1.910494
H	-1.339514	0.392447	-2.689263

H	-0.641551	1.672299	-1.690888
H	0.569785	-1.156715	-2.044539
H	1.212594	0.340197	-2.769398
C	3.228858	-0.613477	-0.537539
C	3.418052	-1.682492	-1.429742
C	4.279305	-0.245126	0.325582
C	4.640338	-2.362107	-1.462381
H	2.622991	-1.995121	-2.108938
C	5.497777	-0.924121	0.284534
H	4.147415	0.584129	1.025855
C	5.680459	-1.985659	-0.609010
H	4.778060	-3.188882	-2.163384
H	6.308098	-0.623426	0.953031
H	6.633862	-2.518405	-0.639136
C	1.941170	2.021566	-0.349504
C	3.016987	2.592687	-1.051344
C	1.034403	2.861057	0.321981
C	3.179819	3.979683	-1.074083
H	3.732888	1.955657	-1.575846
C	1.195227	4.248746	0.288627
H	0.185441	2.436519	0.865389
C	2.270617	4.808713	-0.407094
H	4.020828	4.416351	-1.618242
H	0.480326	4.890502	0.809031
H	2.402861	5.893114	-0.429162
C	-2.668452	-1.411970	-0.779475
C	-3.649356	-1.875502	0.114773
C	-2.458162	-2.090498	-1.989721
C	-4.418472	-2.993689	-0.208589
H	-3.809611	-1.360400	1.065195
C	-3.228820	-3.214536	-2.305649
H	-1.695689	-1.755873	-2.695827
C	-4.208594	-3.666513	-1.418266
H	-5.183587	-3.344384	0.488211
H	-3.060944	-3.736675	-3.250751
H	-4.809344	-4.544529	-1.667618
C	-2.786045	1.363350	0.135394
C	-3.724634	1.796684	-0.817702
C	-2.713971	2.006712	1.381114
C	-4.569024	2.869571	-0.528436
H	-3.803555	1.289776	-1.783161
C	-3.561879	3.081701	1.666027
H	-2.010328	1.656979	2.141236
C	-4.486187	3.514635	0.711512
H	-5.297888	3.202316	-1.271361
H	-3.503856	3.576227	2.638581
H	-5.150255	4.353067	0.935410
C	0.171832	-2.623173	0.818245
C	0.279135	-3.242413	2.217636
H	-0.694627	-2.979294	0.245831
H	1.092766	-2.738851	0.221995
H	0.980113	-4.098612	2.243145
H	-0.698603	-3.616425	2.550943
C	0.762595	-2.184711	3.199308
C	1.825446	-1.379224	2.951807
H	-1.357205	-0.905804	2.326137
H	0.221242	-2.073482	4.145227
H	2.472749	-1.537968	2.082545
H	2.157507	-0.635038	3.683029

^{4}TS7-8A
Geometry with 65 atoms:
Total energy: -2889.257890410

Cr	-0.062191	-0.317530	1.405696
P	1.562769	0.043769	-0.458852
P	-1.610583	0.053533	-0.391073
C	-0.728939	0.505211	-1.975758
C	0.631766	-0.192203	-2.060796
H	-1.356099	0.299324	-2.857080
H	-0.599520	1.598724	-1.925976
H	0.520294	-1.278167	-2.205108
H	1.231787	0.187514	-2.902195
C	2.994808	-1.094017	-0.579056
C	2.726880	-2.467927	-0.732242
C	4.323267	-0.668172	-0.419102
C	3.771697	-3.393411	-0.750511
H	1.697208	-2.823813	-0.837112
C	5.365822	-1.600682	-0.433083
H	4.552524	0.390884	-0.285945
C	5.094452	-2.960914	-0.601762
H	3.552559	-4.456410	-0.877843
H	6.396488	-1.258099	-0.312635
H	5.911896	-3.685893	-0.614205
C	2.209947	1.754201	-0.580614
C	2.964831	2.175357	-1.690827
C	1.916996	2.676998	0.437728
C	3.419147	3.492683	-1.773693
H	3.207682	1.472109	-2.491411
C	2.371665	3.996344	0.351746
H	1.328593	2.367183	1.305721
C	3.123797	4.404113	-0.752920
H	4.006925	3.810109	-2.638424
H	2.137020	4.705308	1.149219
H	3.480968	5.434524	-0.821032
C	-2.497697	-1.519808	-0.729047
C	-3.357588	-2.012209	0.271447
C	-2.322788	-2.265080	-1.906555
C	-4.031397	-3.220514	0.092259
H	-3.506229	-1.441584	1.191638
C	-2.994026	-3.481104	-2.077555
H	-1.672589	-1.908831	-2.707142
C	-3.847641	-3.960795	-1.081472
H	-4.702951	-3.586895	0.872556
H	-2.851071	-4.050665	-2.999124
H	-4.372582	-4.909153	-1.219335
C	-2.909470	1.331681	-0.233537
C	-3.984778	1.382812	-1.136812
C	-2.803360	2.300526	0.775801
C	-4.938338	2.397279	-1.029474
H	-4.084253	0.623838	-1.917517
C	-3.757942	3.316517	0.877649
H	-1.977618	2.254461	1.491063
C	-4.824778	3.365121	-0.024582
H	-5.775780	2.431324	-1.730679
H	-3.671833	4.067359	1.666996
H	-5.573983	4.156503	0.057746
C	-0.741317	-1.552968	2.986502
C	0.095244	-1.066616	4.167959
H	-1.755804	-1.883551	3.240498
H	-0.231577	-2.375649	2.437499
H	0.691083	-1.870337	4.634307
H	-0.541145	-0.631710	4.951983
C	0.979064	0.008628	3.569176
C	2.068861	-0.236987	2.801290
H	-1.548965	-0.337916	1.985798
H	0.666459	1.050364	3.725654
H	2.467582	-1.250807	2.679045
H	2.673622	0.576741	2.392240

^{6}8A
Geometry with 65 atoms:
Total energy: -2889.347183440

Cr	-0.003691	-0.482694	1.475087
P	1.823122	0.146629	-0.205777
P	-1.547225	0.314938	-0.383853
C	-0.424414	0.985228	-1.716532
C	0.910592	0.234942	-1.837042
H	-0.955553	1.004335	-2.681518
H	-0.248714	2.036845	-1.437082
H	0.757732	-0.807476	-2.160393
H	1.546334	0.728266	-2.588910
C	3.260326	-0.940867	-0.521602
C	3.740936	-1.238325	-1.808439
C	3.906218	-1.496179	0.597792
C	4.849250	-2.075883	-1.967905
H	3.262989	-0.818995	-2.695829
C	5.019054	-2.323370	0.434667
H	3.535428	-1.278047	1.603782
C	5.490388	-2.616587	-0.849518
H	5.215032	-2.302783	-2.972372
H	5.516477	-2.745336	1.311316
H	6.357360	-3.269070	-0.978529
C	2.502661	1.847500	-0.027714
C	3.753488	2.219344	-0.547917
C	1.717123	2.813570	0.626781
C	4.202216	3.536961	-0.421976
H	4.383849	1.480705	-1.048542
C	2.164723	4.132208	0.742155
H	0.747372	2.537236	1.051516
C	3.409348	4.495077	0.218268
H	5.178144	3.816254	-0.826718
H	1.543167	4.875320	1.247744
H	3.764336	5.524109	0.313724
C	-2.440203	-1.106900	-1.130754
C	-3.442191	-1.717727	-0.351629
C	-2.130521	-1.650200	-2.387943
C	-4.119030	-2.843435	-0.821042
H	-3.705463	-1.301191	0.624848
C	-2.806132	-2.785223	-2.851730
H	-1.367175	-1.197883	-3.023348
C	-3.797663	-3.384348	-2.071827
H	-4.899507	-3.301793	-0.208728
H	-2.555796	-3.198433	-3.831925
H	-4.323046	-4.269874	-2.437407
C	-2.819433	1.618583	-0.184646
C	-3.839563	1.809113	-1.132504
C	-2.752238	2.460830	0.937357
C	-4.771225	2.834942	-0.959945
H	-3.913135	1.148148	-1.999951
C	-3.683470	3.489996	1.104286
H	-1.973491	2.307710	1.690689
C	-4.693038	3.677001	0.155546
H	-5.564664	2.976543	-1.697951
H	-3.625564	4.140538	1.980413
H	-5.425667	4.477016	0.287836
C	-1.123927	-3.766618	2.067667
C	-1.764429	-2.722785	2.980331
H	-1.865043	-4.521929	1.765975
H	-0.293412	-4.294735	2.562033
H	-2.152154	-3.217578	3.892492
H	-2.656896	-2.295897	2.492455
C	-0.873565	-1.592936	3.439954
C	0.497763	-1.594429	3.452441
H	-0.730015	-3.312010	1.141030
H	-1.390752	-0.776306	3.962061
H	1.077833	-2.456343	3.105490
H	1.051836	-0.823075	3.998672

^{4}9A
Geometry with 77 atoms:
Total energy: -3046.512764200

Cr	-0.065967	-0.695250	1.052269
P	1.730599	0.326419	-0.535891
P	-1.563454	0.346266	-0.611101
C	-0.550531	1.045331	-2.024180
C	0.840537	0.416648	-2.170112
H	-1.120216	0.951381	-2.961275
H	-0.460053	2.122074	-1.814392
H	0.773258	-0.618238	-2.539546
H	1.439792	0.990622	-2.893654
C	3.242023	-0.651951	-0.860711
C	3.693200	-0.976126	-2.151405
C	3.971841	-1.109254	0.252403
C	4.849983	-1.743797	-2.320734
H	3.155236	-0.631898	-3.036424
C	5.132642	-1.864993	0.079565
H	3.630713	-0.874026	1.263576
C	5.571809	-2.186993	-1.209210
H	5.190119	-1.991444	-3.329221
H	5.692010	-2.209278	0.952803
H	6.476528	-2.784080	-1.346439
C	2.298619	2.050912	-0.251083
C	3.618176	2.468465	-0.492467
C	1.360417	2.986512	0.226344
C	3.986645	3.798106	-0.265791
H	4.361983	1.757092	-0.857850
C	1.730456	4.316245	0.440541
H	0.330862	2.682371	0.431255
C	3.046171	4.723590	0.196772
H	5.016122	4.112153	-0.455145
H	0.990171	5.032826	0.804742
H	3.338905	5.761950	0.370242
C	-2.700350	-0.878324	-1.363008
C	-3.985251	-1.060084	-0.823314
C	-2.268882	-1.713478	-2.407403
C	-4.824426	-2.057326	-1.326746
H	-4.337611	-0.418544	-0.012709
C	-3.113488	-2.706722	-2.909325
H	-1.269702	-1.602780	-2.832963
C	-4.391421	-2.882264	-2.369275
H	-5.822893	-2.187274	-0.902265
H	-2.769605	-3.347415	-3.724962
H	-5.049769	-3.661015	-2.761729

C	-2.638270	1.751891	-0.132972
C	-3.428990	2.399247	-1.100558
C	-2.662286	2.209257	1.193808
C	-4.221254	3.490799	-0.743244
H	-3.433655	2.044325	-2.134373
C	-3.458826	3.303665	1.548332
H	-2.069678	1.706134	1.959137
C	-4.235889	3.945521	0.581178
H	-4.833447	3.987270	-1.500074
H	-3.474364	3.650333	2.584363
H	-4.859047	4.799409	0.858094
C	-1.689881	-1.366123	2.166881
C	-1.392157	-2.497328	3.162051
C	-1.053997	-3.847365	2.506809
C	0.391004	-4.003935	2.013493
C	0.927505	-2.873999	1.124919
C	0.089396	-2.418490	-0.035958
H	-2.109686	-0.492429	2.698585
H	-2.473093	-1.702454	1.465415
H	-0.578538	-2.212885	3.859643
H	-2.277755	-2.649309	3.807900
H	-1.243907	-4.661670	3.225569
H	-1.756912	-4.017768	1.672595
H	0.480780	-4.947367	1.448627
H	1.062405	-4.102509	2.884858
H	1.110610	-1.993914	1.849191
H	1.967317	-3.077397	0.823416
H	-0.878558	-2.919114	-0.150425
H	0.623786	-2.371086	-0.993766
C	1.556952	0.314346	3.075657
C	0.365030	0.930623	3.160064
H	2.370741	0.731878	2.475663
H	1.783021	-0.577640	3.668594
H	-0.419995	0.567437	3.827396
H	0.181119	1.874371	2.638051

C	-2.430878	1.958153	-0.047323
C	-3.178034	2.696500	-0.983179
C	-2.387146	2.377964	1.291563
C	-3.864061	3.843403	-0.580935
H	-3.229979	2.372854	-2.025897
C	-3.077140	3.527619	1.689699
H	-1.814912	1.805968	2.024031
C	-3.813168	4.260458	0.754884
H	-4.442734	4.413613	-1.311693
H	-3.040126	3.848317	2.733479
H	-4.352733	5.158319	1.066240
C	1.302022	-2.393248	1.721615
C	0.541321	-2.999609	0.528080
C	-0.345986	-4.208941	0.844790
C	-1.436034	-3.977572	1.897335
C	-2.373001	-2.792428	1.611787
C	-1.828742	-1.425569	2.045713
H	2.330315	-2.150598	1.436184
H	1.313587	-3.118798	2.541183
H	-0.110389	-2.291934	-0.073372
H	1.292511	-3.263784	-0.235049
H	-0.820007	-4.536911	-0.096667
H	0.308753	-5.036665	1.167052
H	-0.976083	-3.844655	2.893525
H	-2.026058	-4.906443	1.966460
H	-2.638423	-2.785459	0.539294
H	-3.327747	-2.977668	2.139546
H	-2.609483	-0.656110	1.904011
H	-1.625502	-1.448351	3.132624
C	0.534030	0.333652	2.827235
C	1.109092	-0.929789	3.178910
H	-0.368931	0.642593	3.364423
H	1.217691	1.148110	2.564107
H	2.194778	-0.993141	3.288230
H	0.564143	-1.546818	3.897618

C	1.585408	2.477887	0.901807
H	0.863529	1.880463	1.468728
H	1.252763	4.267253	2.066926
H	2.918162	5.611182	0.782997
H	4.176496	4.571994	-1.098942
H	3.773774	2.199295	-1.713998
C	0.981910	0.376852	-2.262673
C	-0.322123	1.170762	-2.092894
P	-1.419817	0.518309	-0.718240
C	-2.718380	-0.461240	-1.559613
C	-2.403929	-1.265084	-2.668774
C	-3.369099	-2.111100	-3.221350
C	-4.653084	-2.168323	-2.671119
C	-4.971956	-1.370305	-1.567570
C	-4.011627	-0.521912	-1.011397
H	-4.274368	0.098843	-0.151084
H	-5.976069	-1.405232	-1.137808
H	-5.405440	-2.832335	-3.103309
H	-3.114622	-2.729744	-4.085417
H	-1.403421	-1.247967	-3.106532
C	-2.273990	2.002686	-0.071732
C	-2.853407	2.952237	-0.932248
C	-3.478658	4.084485	-0.407742
C	-3.536843	4.277946	0.977915
C	-2.970033	3.335941	1.840306
C	-2.339425	2.202526	1.316871
H	-1.904879	1.468791	2.002138
H	-3.017922	3.482116	2.922054
H	-4.028594	5.164936	1.384730
H	-3.925929	4.818863	-1.082016
H	-2.820854	2.804618	-2.014590
H	-0.095105	2.213602	-1.823101
H	-0.887561	1.195127	-3.036600
H	1.657732	0.882301	-2.970797
H	0.791395	-0.633453	-2.657103

^{4}TS9-10A
Geometry with 77 atoms:
Total energy: -3046.497379890

Cr	-0.076188	-0.716797	1.142298
P	1.768536	0.292844	-0.489471
P	-1.487854	0.479521	-0.559978
C	-0.449146	1.063265	-2.012371
C	0.893286	0.327226	-2.133304
H	-1.032325	0.965800	-2.940626
H	-0.279189	2.138253	-1.845758
H	0.740564	-0.720854	-2.437191
H	1.529958	0.804792	-2.894714
C	3.319173	-0.639866	-0.746430
C	3.557666	-1.441314	-1.875408
C	4.268470	-0.625891	0.295081
C	4.724002	-2.210399	-1.959876
H	2.846386	-1.469424	-2.703236
C	5.432494	-1.389509	0.202908
H	4.101442	-0.004042	1.179405
C	5.661591	-2.186851	-0.924653
H	4.901399	-2.825641	-2.845350
H	6.164036	-1.363008	1.014302
H	6.572136	-2.786518	-0.995351
C	2.270333	2.043696	-0.250789
C	3.487613	2.546877	-0.742748
C	1.376610	2.918720	0.393491
C	3.801044	3.899780	-0.589810
H	4.195293	1.881917	-1.242937
C	1.689551	4.273436	0.533502
H	0.427942	2.549818	0.787404
C	2.903655	4.765077	0.045661
H	4.751379	4.280588	-0.972019
H	0.982591	4.942095	1.030582
H	3.152775	5.822690	0.162075
C	-2.710844	-0.681458	-1.276881
C	-4.047155	-0.680857	-0.845772
C	-2.276837	-1.678902	-2.168255
C	-4.932988	-1.659825	-1.304994
H	-4.401607	0.082613	-0.150323
C	-3.166293	-2.653730	-2.625537
H	-1.240456	-1.705114	-2.512339
C	-4.496373	-2.647858	-2.192100
H	-5.971165	-1.649104	-0.964673
H	-2.818766	-3.420666	-3.322001
H	-5.191530	-3.412234	-2.547299

^{4}10A
Geometry with 77 atoms:
Total energy: -3046.526642130

Cr	0.208523	-0.727746	0.946585
C	-0.033485	-2.543784	0.027722
C	-1.355492	-3.304448	0.179355
C	-1.668886	-3.933023	1.548911
C	-2.307750	-2.996765	2.586562
C	-1.439026	-1.822265	3.036524
C	-0.167951	-2.198706	3.805812
C	0.902517	-1.103269	3.809083
C	1.600332	-0.960093	2.445574
H	2.186865	-1.866617	2.209155
H	2.310137	-0.112224	2.451867
H	1.648258	-1.327498	4.595135
H	0.442080	-0.142897	4.114531
H	0.272923	-3.115944	3.381613
H	-0.470148	-2.452844	4.835703
H	-2.034615	-1.113598	3.636762
H	-1.242288	-1.213597	2.112795
H	-2.579166	-3.580889	3.483472
H	-3.255685	-2.606481	2.176380
H	-0.755834	-4.397771	1.959752
H	-2.375089	-4.764301	1.389072
H	-2.203399	-2.668332	-0.128697
H	-1.341432	-4.125269	-0.563170
H	0.823547	-3.140844	0.389351
H	0.145860	-2.322392	-1.041179
P	1.846291	0.179336	-0.626681
C	3.384097	-0.746564	-0.934578
C	3.375453	-1.860508	-1.793581
C	4.530860	-2.627251	-1.959527
C	5.699018	-2.298563	-1.264525
C	5.709032	-1.200135	-0.399570
C	4.558145	-0.426817	-0.229691
H	4.580168	0.428734	0.448745
H	6.618471	-0.940695	0.147740
H	6.601665	-2.899937	-1.396354
H	4.516776	-3.486563	-2.634240
H	2.470177	-2.142591	-2.335685
C	2.283690	1.888949	-0.164330
C	3.218585	2.649572	-0.886998
C	3.445387	3.982904	-0.540023
C	2.738248	4.566189	0.519050
C	1.805791	3.815072	1.240566

^{4}10A'
Geometry with 77 atoms:
Total energy: -3046.526036560

Cr	-0.056074	-0.585302	0.956814
C	-1.157159	-2.338005	0.799597
C	-0.498809	-2.664741	2.104335
C	-1.365269	-2.653701	3.376573
C	-2.372176	-1.497786	3.512327
C	-1.895526	-0.056604	3.269010
C	-0.795631	0.535339	4.162700
C	0.642840	0.060074	3.910469
C	1.137844	0.252266	2.470454
H	2.193360	-0.057688	2.383649
H	1.114518	1.325483	2.187825
H	0.749864	-0.997193	4.206438
H	1.302941	0.614982	4.604743
H	-1.067618	0.356719	5.217944
H	-0.815951	1.631903	4.029056
H	-2.786149	0.589411	3.345631
H	-1.616618	0.075479	2.193771
H	-2.804675	-1.545870	4.526213
H	-3.215359	-1.680091	2.824671
H	-0.697444	-2.677452	4.252540
H	-1.934834	-3.597663	3.406741
H	0.098813	-3.590938	2.061050
H	0.344231	-1.903203	2.296654
H	-0.821515	-2.934630	-0.061484
H	-2.249852	-2.251844	0.812487
P	1.767065	-0.017850	-0.659690
C	2.677597	-1.517734	-1.184687
C	3.566403	-1.486509	-2.274935
C	4.247953	-2.642827	-2.657324
C	4.051026	-3.839357	-1.957130
C	3.174172	-3.877311	-0.870023
C	2.490373	-2.720424	-0.484242
H	1.809053	-2.755451	0.369219
H	3.020553	-4.808467	-0.319572
H	4.586285	-4.742709	-2.259798
H	4.938690	-2.610493	-3.503422
H	3.740544	-0.554938	-2.819525
C	3.023662	1.229227	-0.199361
C	2.624052	2.569955	-0.046906
C	3.535455	3.530764	0.394078
C	4.850366	3.163818	0.700226
C	5.249313	1.831642	0.563130

C	4.342309	0.864971	0.118122
H	4.668779	-0.171969	0.016872
H	6.274374	1.538758	0.802955
H	5.562115	3.916109	1.048577
H	3.215419	4.569967	0.502552
H	1.597199	2.872830	-0.266045
C	0.976279	0.629990	-2.222033
C	-0.393921	-0.020516	-2.445614
P	-1.447338	0.212185	-0.930790
C	-3.067265	-0.551420	-1.286279
C	-3.236894	-1.529523	-2.278668
C	-4.480199	-2.148000	-2.448586
C	-5.558181	-1.800083	-1.631054
C	-5.393823	-0.826845	-0.638397
C	-4.156007	-0.206691	-0.463900
H	-4.039054	0.555987	0.311180
H	-6.234621	-0.548156	0.001471
H	-6.527723	-2.285181	-1.767167
H	-4.603717	-2.904836	-3.227109
H	-2.408966	-1.819623	-2.928139
C	-1.769636	2.019526	-0.897729
C	-2.539798	2.634878	-1.900993
C	-2.741412	4.015958	-1.880983
C	-2.180789	4.794961	-0.861100
C	-1.419541	4.190171	0.142423
C	-1.215265	2.806340	0.125381
H	-0.620219	2.343082	0.915985
H	-0.985760	4.792673	0.944106
H	-2.344465	5.875268	-0.847410
H	-3.342257	4.487631	-2.662347
H	-2.993111	2.033029	-2.692999
H	-0.900670	0.409130	-3.323924
H	-0.287364	-1.104354	-2.614244
H	0.873284	1.720411	-2.109755
H	1.643750	0.455297	-3.079022
C	2.801042	0.003593	-1.256122
C	4.035310	0.552288	-0.867573
C	2.779269	-1.240094	-1.914864
C	5.225287	-0.126651	-1.145804
H	4.074186	1.510794	-0.346336
C	3.971355	-1.911224	-2.193393
H	1.831361	-1.697186	-2.211789
C	5.197005	-1.356854	-1.808191
H	6.179018	0.310705	-0.840856
H	3.942948	-2.872897	-2.711360
H	6.128778	-1.884919	-2.024469
C	1.848987	0.025530	2.342864
C	2.845260	-0.936461	3.004357
H	2.388593	0.618483	1.592893
H	1.439683	0.734310	3.086464
C	-1.578184	-1.302874	2.158690
C	3.412951	-1.994949	2.048942
H	3.683993	-0.353541	3.423606
H	2.374969	-1.433633	3.871587
C	-0.362007	-1.858649	2.710269
H	-2.123214	-0.550570	2.743458
H	-2.235747	-1.964281	1.583308
C	2.374043	-2.932012	1.414306
H	3.973356	-1.492540	1.241920
H	4.147880	-2.606828	2.600873
C	-0.009141	-3.304115	2.344305
H	0.774331	-1.037579	2.410773
H	-0.162087	-1.622395	3.768005
C	1.472293	-3.693355	2.414641
H	2.907632	-3.644048	0.764900
H	1.738018	-2.346675	0.719832
H	-0.594322	-3.960098	3.013056
H	-0.382114	-3.515816	1.326455
H	1.542795	-4.777212	2.229556
H	1.838770	-3.549552	3.445341
C	-3.715195	0.029535	-0.171728
C	-4.620433	-0.508659	-1.102337
C	-4.194157	0.851244	0.862269
C	-5.982779	-0.218334	-1.000853
H	-4.263184	-1.162056	-1.902240
C	-5.557486	1.144502	0.957191
H	-3.498804	1.259088	1.602403
C	-6.452110	0.609503	0.025535
H	-6.682672	-0.641241	-1.725779
H	-5.922269	1.784172	1.764591
H	-7.519125	0.832757	0.102137
C	0.912255	-0.346861	3.562759
C	0.041401	-1.395152	3.417538
C	0.370565	-2.774238	2.889498
C	1.670754	-2.957716	2.095039
C	1.658585	-2.337391	0.693607
C	2.940102	-2.542167	-0.121564
H	1.962040	-0.423342	3.261543
H	0.643315	0.522439	4.173684
H	-0.944177	-1.312829	3.896451
H	3.804917	-2.157005	0.449209
H	0.397092	-3.434341	3.778332
H	-0.480407	-3.146499	2.292604
H	1.850192	-4.040740	2.004284
H	2.526347	-2.561715	2.670028
H	0.797024	-2.732350	0.128446
H	1.495495	-1.244713	0.780441
H	2.883570	-1.914908	-1.029132
C	3.207890	-3.990219	-0.543926
H	3.326442	-4.627005	0.349803
H	2.320772	-4.378062	-1.077393
C	4.445319	-4.130840	-1.429557
H	4.621158	-5.179523	-1.718660
H	4.344031	-3.541822	-2.357232
H	5.350747	-3.772763	-0.910770

[4]TS10-11A

Geometry with 77 atoms:

Total energy: -3046.511230440

Cr	-0.003817	-0.375595	1.109909
P	-1.848914	0.166412	-0.464635
P	1.212559	0.766834	-0.763797
C	0.136868	0.796666	-2.284295
C	-1.261357	1.258750	-1.863989
H	0.574791	1.455923	-3.048876
H	0.104473	-0.222674	-2.702312
H	-1.235212	2.299720	-1.507124
H	-1.975296	1.212664	-2.699792
C	-3.275052	1.031295	0.286556
C	-3.149803	2.390226	0.630666
C	-4.441770	0.336556	0.648985
C	-4.184041	3.044426	1.304153
H	-2.245861	2.952156	0.379992
C	-5.472018	0.996795	1.324312
H	-4.553717	-0.720849	0.400949
C	-5.347526	2.350205	1.651162
H	-4.079367	4.101924	1.558873
H	-6.377388	0.448037	1.595052
H	-6.155839	2.863762	2.177230
C	-2.500865	-1.281236	-1.384462
C	-3.607588	-1.154525	-2.243911
C	-1.831380	-2.512838	-1.306818
C	-4.035495	-2.245002	-3.003255
H	-4.142261	-0.203838	-2.315543
C	-2.256999	-3.601580	-2.074322
H	-0.974876	-2.630644	-0.638856
C	-3.360451	-3.468869	-2.920984
H	-4.899545	-2.139556	-3.663782
H	-1.727627	-4.554896	-2.005148
H	-3.697514	-4.319747	-3.518031
C	1.537127	2.547018	-0.468473
C	1.078627	3.150674	0.713842
C	2.185248	3.336459	-1.436410
C	1.260555	4.520986	0.926628
H	0.582476	2.551420	1.480654
C	2.369626	4.703003	-1.219304
H	2.555569	2.882041	-2.358888
C	1.906794	5.296976	-0.038790
H	0.900817	4.979503	1.850845
H	2.877159	5.308300	-1.974261
H	2.053512	6.366901	0.128168

[6]11A

Geometry with 77 atoms:

Total energy: -3046.581253960

Cr	-0.254736	0.184786	1.623538
P	0.880278	1.657809	-0.136961
P	-1.910762	-0.269879	-0.282611
C	-1.362133	0.853176	-1.669632
C	0.162201	1.024940	-1.744829
H	-1.769414	0.496505	-2.629443
H	-1.849180	1.821058	-1.466612
H	0.659713	0.063855	-1.949968
H	0.424130	1.715763	-2.561568
C	2.690750	1.449004	-0.320350
C	3.332256	1.248290	-1.554606
C	3.460497	1.462139	0.857171
C	4.717226	1.060287	-1.605193
H	2.762188	1.237412	-2.485514
C	4.844176	1.283943	0.802003
H	2.971043	1.608509	1.824657
C	5.474080	1.077877	-0.430219
H	5.206223	0.900496	-2.569296
H	5.431562	1.298198	1.723339
H	6.555655	0.928706	-0.473908
C	0.554182	3.461810	-0.223673
C	1.440101	4.361240	-0.839682
C	-0.650526	3.942514	0.319016
C	1.118265	5.718829	-0.916140
H	2.384853	4.004072	-1.256519
C	-0.973353	5.299435	0.231035
H	-1.341235	3.254097	0.815069
C	-0.087842	6.188978	-0.385357
H	1.814320	6.413815	-1.392352
H	-1.913666	5.663636	0.652132
H	-0.334898	7.251639	-0.447348
C	-1.737648	-1.986393	-0.912889
C	-2.164216	-3.024700	-0.062163
C	-1.121108	-2.315684	-2.130173
C	-1.980720	-4.359433	-0.423075
H	-2.647668	-2.786812	0.890026
C	-0.928072	-3.656406	-2.484231
H	-0.782649	-1.538022	-2.816936
C	-1.353718	-4.679196	-1.633575
H	-2.323371	-5.154058	0.244254
H	-0.443270	-3.898968	-3.433038
H	-1.200552	-5.724413	-1.912514

[6]1B

Geometry with 67 atoms:

Total energy: -3039.804529210

Cr	0.007016	-0.072959	1.679833
P	-1.652999	0.198058	-0.223327
P	1.665173	-0.132239	-0.229594
O	-0.107809	2.585865	0.410039
O	0.119041	-2.533328	0.397915
C	0.719736	0.361194	-1.761370
C	-0.698882	-0.222757	-1.773195
H	0.686612	1.461294	-1.762101
H	1.267549	0.034684	-2.658851
H	-1.247411	0.138893	-2.656575
H	-0.662963	-1.322491	-1.822392
C	-2.186048	1.936255	-0.503982
C	-3.428991	2.272735	-1.057231
C	-1.299378	2.974946	-0.131245
C	-3.792948	3.608656	-1.249520
H	-4.124413	1.478391	-1.338075
C	-1.659751	4.314196	-0.326061
C	-2.905061	4.621731	-0.884420
H	-4.765172	3.853667	-1.682217
H	-0.982663	5.120678	-0.045751
H	-3.177807	5.669816	-1.030608
C	-3.185764	-0.797157	-0.322744
C	-3.623210	-1.447043	-1.489004
C	-3.937403	-0.931942	0.859329
C	-4.789664	-2.219221	-1.468612
H	-3.064451	-1.357508	-2.422372
C	-5.107266	-1.693564	0.873122
H	-3.601738	-0.436548	1.775522
C	-5.533108	-2.342556	-0.291441
H	-5.120208	-2.723103	-2.380319
H	-5.684966	-1.786546	1.796046
H	-6.444710	-2.945003	-0.280333
C	2.167904	-1.867098	-0.584086
C	3.382757	-2.196683	-1.200386
C	1.285555	-2.909441	-0.211889
C	3.722053	-3.527964	-1.457447
H	4.074797	-1.399460	-1.481911
C	1.620840	-4.244074	-0.471329
C	2.837457	-4.544228	-1.093184
H	4.672130	-3.767046	-1.939865
H	0.947029	-5.053184	-0.190983
H	3.090432	-5.589076	-1.289388

C	3.210223	0.845296	-0.279603
C	3.666560	1.529431	-1.418806
C	3.950220	0.931689	0.914129
C	4.841121	2.286980	-1.360259
H	3.114698	1.479972	-2.359232
C	5.128206	1.678957	0.965641
H	3.598071	0.410636	1.809680
C	5.573460	2.361653	-0.172018
H	5.186495	2.818281	-2.250634
H	5.696940	1.734460	1.897125
H	6.491412	2.953082	-0.131168
C	0.873824	3.557350	0.749786
H	1.736990	3.000676	1.136940
H	1.191052	4.134187	-0.135248
H	0.507537	4.247799	1.528337
C	-0.879680	-3.508120	0.681058
H	-0.520748	-4.254958	1.408879
H	-1.730013	-2.963038	1.110108
H	-1.212387	-4.018165	-0.238195
C	-0.691407	-0.322161	3.876797
C	0.681824	-0.364847	3.878110
H	-1.233141	0.602915	4.104416
H	-1.287837	-1.241299	3.847542
H	1.221745	-1.318035	3.847396
H	1.277203	0.526203	4.107603

^{6}2B

Geometry with 73 atoms:

Total energy: -3118.393763650

Cr	-0.003093	-0.005030	1.563317
P	-1.668670	0.127365	-0.336161
P	1.654829	-0.119353	-0.351555
O	-0.281617	2.686180	-0.166625
O	0.274350	-2.681643	-0.225068
C	0.706620	0.271657	-1.917140
C	-0.734419	-0.255071	-1.912565
H	0.708859	1.368143	-1.991827
H	1.249171	-0.130603	-2.786436
H	-1.284871	0.155039	-2.773214
H	-0.737824	-1.350678	-1.996046
C	-2.413793	1.788177	-0.622244
C	-3.768399	1.973818	-0.930753
C	-1.588126	2.928911	-0.472446
C	-4.302298	3.256019	-1.094809
H	-4.419294	1.104138	-1.040720
C	-2.120021	4.214214	-0.635126
C	-3.475166	4.369544	-0.946844
H	-5.360100	3.379598	-1.336464
H	-1.489780	5.096082	-0.523000
H	-3.880590	5.376514	-1.072682
C	-3.098466	-1.020286	-0.367440
C	-3.586609	-1.624023	-1.538950
C	-3.711733	-1.321635	0.862209
C	-4.661040	-2.516827	-1.476569
H	-3.136432	-1.402903	-2.508730
C	-4.792608	-2.204624	0.920426
H	-3.337791	-0.862731	1.782386
C	-5.265654	-2.808000	-0.249702
H	-5.030286	-2.983854	-2.393000
H	-5.262858	-2.426638	1.881590
H	-6.106163	-3.504974	-0.205586
C	2.408786	-1.774803	-0.645690
C	3.768995	-1.954559	-0.932348
C	1.585695	-2.919412	-0.512309
C	4.310631	-3.234459	-1.089528
H	4.418301	-1.082237	-1.029587
C	2.125023	-4.202364	-0.668106
C	3.485939	-4.351695	-0.956975
H	5.372871	-3.353336	-1.313449
H	1.496466	-5.086860	-0.567789
H	3.897701	-5.356810	-1.076918
C	3.079801	1.034326	-0.385138
C	3.557626	1.646082	-1.556668
C	3.701416	1.330463	0.841627
C	4.629398	2.542218	-1.497189
H	3.101895	1.428112	-2.524550
C	4.779622	2.216996	0.896899
H	3.336436	0.864446	1.761697
C	5.241906	2.828770	-0.273179
H	4.990607	3.015137	-2.413813
H	5.256307	2.435102	1.855789
H	6.080374	3.528337	-0.231349
C	0.623434	3.767529	0.003412
H	1.599922	3.320732	0.227798
H	0.712200	4.367677	-0.918082
H	0.319712	4.422947	0.837322
C	-0.629583	-3.766102	-0.070329
H	-0.335559	-4.422887	0.765924
H	-1.610033	-3.321902	0.142122
H	-0.703629	-4.364442	-0.994284
C	0.654208	1.774436	3.172920
C	-0.702360	1.792297	3.114532
H	1.185256	1.257695	3.978953
H	1.263842	2.376392	2.492119
H	-1.235678	2.407240	2.382706
H	-1.313474	1.293440	3.873813
C	0.784956	-1.876947	3.029622
C	-0.568459	-1.882818	3.113096
H	1.316380	-2.453774	2.266302
H	1.401257	-1.390176	3.792361
H	-1.090719	-1.399028	3.945065
H	-1.184393	-2.469678	2.425106

^{4}TS2_3B

Geometry with 73 atoms:

Total energy: -3118.363816240

Cr	-0.000010	-0.000082	1.425369
P	1.522529	-0.122697	-0.530412
P	-1.522532	0.122760	-0.530409
O	0.193465	-2.466274	0.748085
O	-0.193415	2.466156	0.748367
C	-0.698244	-0.309966	-2.148047
C	0.698252	0.310249	-2.147996
H	-0.631788	-1.407289	-2.214767
H	-1.310354	0.043400	-2.991982
H	1.310371	-0.042995	-2.991975
H	0.631788	1.407580	-2.214561
C	1.930105	-1.896898	-0.771998
C	2.931662	-2.298454	-1.670229
C	1.193044	-2.890231	-0.084715
C	3.223322	-3.647565	-1.875334
H	3.500168	-1.536786	-2.209353
C	1.489365	-4.246833	-0.283496
C	2.500820	-4.615437	-1.174109
H	4.009605	-3.939340	-2.574415
H	0.938053	-5.021772	0.247462
H	2.720428	-5.676135	-1.318613
C	3.108815	0.790117	-0.547887
C	3.126759	2.132288	-0.970244
C	4.282407	0.228944	-0.014101
C	4.298984	2.887406	-0.879182
H	2.226751	2.602341	-1.372517
C	5.451783	0.988419	0.074659
H	4.288299	-0.805590	0.334045
C	5.464686	2.317778	-0.358236
H	4.300378	3.925739	-1.220036
H	6.357754	0.536625	0.485983
H	6.381129	2.908789	-0.289504
C	-1.930112	1.896997	-0.771737
C	-2.931693	2.298690	-1.669881
C	-1.193035	2.890231	-0.084326
C	-3.223369	3.647832	-1.874764
H	-3.500203	1.537107	-2.209119
C	-1.489376	4.246861	-0.282878
C	-2.500861	4.615599	-1.173402
H	-4.009671	3.939710	-2.573780
H	-0.938055	5.021719	0.248190
H	-2.720483	5.676318	-1.317728
C	-3.108813	-0.790063	-0.548003
C	-3.126737	-2.132189	-0.970502
C	-4.282416	-0.228960	-0.014168
C	-4.298956	-2.887328	-0.879538
H	-2.226721	-2.602193	-1.372814
C	-5.451786	-0.988457	0.074495
H	-4.288320	0.805535	0.334092
C	-5.464671	-2.317769	-0.358546
H	-4.300335	-3.925625	-1.220503
H	-6.357766	-0.536717	0.485859
H	-6.381109	-2.908795	-0.289891
C	-0.588950	-3.422932	1.459009
H	-1.348592	-2.854194	2.008014
H	-1.096817	-4.117322	0.770969
H	0.029359	-3.991826	2.172813
C	0.589056	3.422715	1.459364
H	-0.029193	3.991494	2.173311
H	1.348756	2.853902	2.008210
H	1.096850	4.117215	0.771381
C	-1.840158	-0.003452	2.410761
C	-0.970236	-0.209879	3.548365
H	-2.361261	0.961011	2.348291
H	-2.466709	-0.847967	2.104741
H	-0.912404	-1.247662	3.898316
H	-1.086940	0.482829	4.387544
C	1.840125	0.003181	2.410788
C	0.970188	0.209511	3.548398
H	2.361215	-0.961283	2.348230
H	2.466690	0.847718	2.104856
H	0.912355	1.247265	3.898439
H	1.086877	-0.483271	4.387518

^{4}3B

Geometry with 73 atoms:

Total energy: -3118.393054210

Cr	-0.024917	-0.109038	1.240661
C	1.407709	-0.295676	2.742944
C	0.675542	-0.178339	4.086864
C	-0.686906	-0.870429	3.971283
C	-1.427877	-0.291885	2.760906
H	-1.734773	0.753493	2.959352
H	-2.344925	-0.852866	2.507090
H	-1.267596	-0.778480	4.910016
H	-0.522257	-1.955262	3.824207
H	1.266559	-0.587799	4.929110
H	0.507407	0.888809	4.329193
H	1.782003	-1.327819	2.598596
H	2.286592	0.370676	2.676631
P	1.586009	0.016211	-0.709664
C	3.191073	0.879960	-0.785169
C	3.508426	1.823646	-1.776312
C	4.736647	2.493021	-1.739412
C	5.654824	2.226692	-0.720904
C	5.344487	1.285583	0.268133
C	4.119269	0.619266	0.241499
H	3.884567	-0.113995	1.016635
H	6.059706	1.071119	1.065892
H	6.613590	2.750251	-0.697458
H	4.976092	3.222406	-2.517085
H	2.813239	2.044024	-2.588224
C	1.992483	-1.771716	-0.798012
C	3.072927	-2.257718	-1.550952
C	3.394666	-3.615229	-1.556499
C	2.635712	-4.502395	-0.790079
C	1.556447	-4.045979	-0.028232
C	1.233306	-2.685102	-0.035379
O	0.158364	-2.193286	0.698176
C	-0.868909	-3.120485	1.107733
H	-1.721633	-2.517493	1.429663
H	-0.517345	-3.740087	1.944543
H	-1.162117	-3.751009	0.255532
H	0.989445	-4.755086	0.573516
H	2.884355	-5.566079	-0.773228
H	4.238597	-3.976625	-2.147630
H	3.676923	-1.554162	-2.129476
C	0.697445	0.412231	-2.299205
C	-0.703442	-0.210545	-2.319383
P	-1.594448	0.096980	-0.713774
C	-3.239173	-0.674676	-0.869894
C	-3.567603	-1.578163	-1.894358
C	-4.820462	-2.201399	-1.903744
C	-5.750986	-1.929707	-0.897775
C	-5.428563	-1.030028	0.125423
C	-4.179358	-0.409601	0.144624
H	-3.931931	0.287496	0.949221
H	-6.152702	-0.813168	0.914401
H	-6.728667	-2.417355	-0.910019
H	-5.069151	-2.899374	-2.706923
H	-2.860281	-1.803819	-2.694550
C	-1.890593	1.901271	-0.645681
C	-2.815718	2.533491	-1.491451
C	-3.056761	3.903778	-1.400355
C	-2.371178	4.652982	-0.441530
C	-1.446254	4.049838	0.414954
C	-1.199176	2.675176	0.311851

O	-0.273547	2.039623	1.131760
C	0.563397	2.857978	1.975698
H	1.306836	2.190303	2.416041
H	1.072872	3.621903	1.370162
H	-0.036481	3.325713	2.769832
H	-0.937684	4.660852	1.158216
H	-2.556943	5.725508	-0.347314
H	-3.779848	4.381294	-2.064602
H	-3.362387	1.932235	-2.222792
H	-0.633344	-1.305543	-2.426697
H	-1.289493	0.170974	-3.170273
H	1.287145	0.081088	-3.168295
H	0.621302	1.511186	-2.342564

^{4}4B
Geometry with 79 atoms:
Total energy: -3196.971720560

Cr	-0.354897	-0.477958	1.232502
P	-1.818739	-0.046036	-0.646281
P	1.409285	0.068506	-0.678891
O	-0.996695	1.765765	1.535443
O	3.611693	-0.983376	0.877696
C	0.416322	0.420951	-2.221829
C	-0.918798	-0.330928	-2.243199
H	1.014325	0.211770	-3.121885
H	0.239378	1.507502	-2.206579
H	-0.766158	-1.417459	-2.331919
H	-1.547648	-0.012504	-3.089394
C	-2.047645	1.768278	-0.611841
C	-2.628505	2.473307	-1.678250
C	-2.725931	3.863945	-1.645840
C	-2.235363	4.562301	-0.537517
C	-1.657690	3.882117	0.536545
C	-1.567633	2.485328	0.499026
H	-1.276703	4.441599	1.391045
H	-2.300038	5.652420	-0.504987
H	-3.181656	4.401838	-2.479615
H	-3.013975	1.922058	-2.539834
C	-3.472464	-0.780850	-0.831698
C	-4.562775	-0.210159	-0.152569
C	-5.816024	-0.823394	-0.199156
C	-5.991627	-2.010622	-0.917668
C	-4.909554	-2.583767	-1.592412
C	-3.652075	-1.976231	-1.549211
H	-2.816869	-2.446229	-2.072848
H	-5.042198	-3.511521	-2.154080
H	-6.973051	-2.489631	-0.951376
H	-6.659258	-0.371833	0.328977
H	-4.434266	0.717158	0.410169
C	2.442125	-1.381831	-1.119977
C	2.219929	-2.168301	-2.258710
C	2.990185	-3.307367	-2.513669
C	4.001823	-3.666635	-1.623261
C	4.246894	-2.901237	-0.478655
C	3.462586	-1.770556	-0.218227
H	5.041518	-3.195653	0.206455
H	4.613066	-4.552033	-1.814135
H	2.799620	-3.905327	-3.407182
H	1.439008	-1.898622	-2.971017
C	2.558130	1.498569	-0.621429
C	3.773679	1.520859	-1.323195
C	4.591090	2.652685	-1.272287
C	4.202764	3.770127	-0.524778
C	2.993818	3.752930	0.177366
C	2.176303	2.619830	0.134331
H	1.238463	2.605337	0.694402
H	2.687950	4.622771	0.764282
H	4.844932	4.653657	-0.488521
H	5.536226	2.663156	-1.821060
H	4.085025	0.651628	-1.907677
C	-0.238062	-2.505872	0.767634
C	-1.042602	-3.262821	1.831965
C	-2.322890	-2.478490	2.143212
C	-1.953183	-1.023220	2.449516
H	-1.547319	-0.931389	3.477688
H	-2.819944	-0.340769	2.386022
H	-2.982887	-2.511307	1.258953
H	-2.894371	-2.953865	2.963858
H	-0.443694	-3.357424	2.756559
H	-1.272154	-4.300218	1.519751
H	0.807205	-2.849669	0.686457
H	-0.691995	-2.657164	-0.230179
C	1.374537	-1.171499	3.113879
C	1.549720	0.149455	2.931986
H	1.047475	0.881322	3.569812
H	2.270918	0.531625	2.206182
H	0.711815	-1.561665	3.890498
H	1.936271	-1.898768	2.524673
C	-1.171064	2.286199	2.866363
H	-0.400023	3.037449	3.096566
H	-1.085600	1.440411	3.557353
H	-2.172263	2.728602	2.974500
C	4.709382	-1.183247	1.755143
H	4.660624	-2.166230	2.254271
H	4.645135	-0.394506	2.516016
H	5.670072	-1.090803	1.220698

^{4}TS4-5B
Geometry with 79 atoms:
Total energy: -3196.956552950

Cr	-0.506886	-0.573579	1.362666
P	-1.727180	-0.084118	-0.756132
P	1.429886	-0.289513	-0.274833
C	0.755662	0.046948	-1.990942
C	-0.637331	-0.562677	-2.178487
H	0.712726	1.135669	-2.134467
H	1.466828	-0.340835	-2.731768
H	-1.086087	-0.241176	-3.131490
H	-0.588686	-1.663912	-2.185627
C	-1.783888	1.743816	-0.834267
C	-2.343382	2.412559	-1.934534
C	-1.242417	2.500069	0.226594
C	-2.362827	3.805238	-1.998180
H	-2.779002	1.825227	-2.747026
C	-1.262909	3.901241	0.168011
C	-1.819423	4.541335	-0.942090
H	-2.801022	4.311963	-2.860321
H	-0.845081	4.504225	0.971812
H	-1.827146	5.633524	-0.974003
C	-3.415412	-0.635762	-1.164255
C	-3.651575	-1.702790	-2.046832
C	-4.496636	-0.057456	-0.473669
C	-4.952471	-2.178121	-2.238286
H	-2.827674	-2.175476	-2.585286
C	-5.792593	-0.535880	-0.670456
H	-4.326023	0.772119	0.217746
C	-6.022904	-1.598528	-1.551673
H	-5.128061	-3.006883	-2.928472
H	-6.626600	-0.078491	-0.132675
H	-7.037769	-1.974250	-1.702377
C	2.624081	-1.655159	-0.502824
C	2.477695	-2.856440	0.204044
C	3.724133	-1.507126	-1.388413
C	3.395476	-3.899773	0.054041
H	1.632245	-2.974963	0.880048
C	4.648523	-2.551641	-1.533168
C	4.477235	-3.738136	-0.812811
H	3.264420	-4.828854	0.612282
H	5.498170	-2.449795	-2.208305
H	5.204609	-4.544355	-0.937582
C	2.457903	1.169375	0.169267
C	2.118101	2.470200	-0.234828
C	3.552731	0.989777	1.033372
C	2.864152	3.567359	0.207076
H	1.269104	2.649130	-0.896357
C	4.294429	2.088149	1.474458
H	3.835849	-0.014560	1.357680
C	3.953121	3.381180	1.063510
H	2.590342	4.572402	-0.124279
H	5.146626	1.931367	2.140445
H	4.536523	4.239101	1.406550
O	-0.695598	1.814419	1.294332
O	3.801873	-0.332819	-2.051856
C	-0.214780	2.582514	2.407059
H	-1.025246	3.192282	2.835166
H	0.130411	1.870886	3.160618
H	0.630424	3.218102	2.104987
C	4.930537	-0.039178	-2.860077
H	4.785681	0.985851	-3.226271
H	5.866266	-0.083945	-2.276996
H	5.002754	-0.723657	-3.722887
C	-0.940817	-2.588072	1.146476
C	-2.404592	-2.824516	1.524629
H	-0.705874	-2.967406	0.136243
H	-0.272946	-3.108006	1.858398
H	-2.635477	-3.903157	1.613181
H	-3.067454	-2.445149	0.729871
C	-2.736297	-2.105732	2.836538
C	-2.183742	-0.686642	2.845277
H	-3.828613	-2.089984	3.009621
H	-2.308864	-2.665591	3.688024
H	-2.443649	-0.134169	3.755367
H	-2.599975	-0.086544	2.010294
C	-0.186216	-0.749010	3.711905
C	0.971514	-0.699033	2.906067
H	-0.427091	0.115930	4.334521
H	-0.484764	-1.701286	4.156037
H	1.529640	-1.621235	2.721679
H	1.574478	0.214913	2.891116

^{4}5B
Geometry with 79 atoms:
Total energy: -3196.999213950

Cr	-0.418902	-0.758669	1.117685
P	1.336886	-0.088887	-0.501959
P	-1.893636	0.051458	-0.782007
O	3.633519	0.297205	-2.320798
O	-0.805937	1.492444	1.585184
C	-0.831486	-0.010165	-2.309451
C	0.532009	0.630463	-2.027650
H	-0.714099	-1.072756	-2.578153
H	-1.336413	0.494390	-3.148450
H	1.219947	0.503378	-2.874504
H	0.415764	1.712046	-1.871207
C	2.491882	-1.361822	-1.107582
C	2.342892	-2.699787	-0.717030
C	3.234776	-3.680355	-1.159171
C	4.291348	-3.315705	-1.995747
C	4.462306	-1.988396	-2.402254
C	3.561880	-1.005096	-1.968715
H	5.292198	-1.728094	-3.058929
H	4.999674	-4.071738	-2.343974
H	3.107144	-4.718371	-0.845834
H	1.520143	-2.969144	-0.054942
C	2.373335	1.233547	0.233823
C	2.002123	2.586296	0.182380
C	2.752973	3.550388	0.862345
C	3.878120	3.175210	1.602243
C	4.251697	1.828153	1.657848
C	3.504123	0.862041	0.981387
H	3.804483	-0.186889	1.033670
H	5.131087	1.525931	2.231917
H	4.464618	3.930266	2.131361
H	2.455350	4.600712	0.807922
H	1.126822	2.909814	-0.383233
C	-2.026989	1.847177	-0.448247
C	-2.659058	2.723043	-1.345486
C	-2.684474	4.097828	-1.114002
C	-2.061650	4.606931	0.028657
C	-1.429628	3.757818	0.940487
C	-1.417181	2.374779	0.710279
H	-0.945486	4.186061	1.816054
H	-2.063904	5.682406	0.221492
H	-3.181137	4.766760	-1.819671
H	-3.141693	2.312257	-2.236457
C	-3.556717	-0.506517	-1.282087
C	-4.672905	-0.107548	-0.523471
C	-5.944888	-0.589246	-0.836665
C	-6.117630	-1.479741	-1.902380
C	-5.012306	-1.885755	-2.654620
C	-3.735486	-1.405222	-2.347946
H	-2.886103	-1.736393	-2.948993
H	-5.140983	-2.580139	-3.488490
H	-7.114132	-1.856001	-2.145703
H	-6.806289	-0.266681	-0.246626
H	-4.550644	0.591551	0.308210
C	-0.355675	2.004975	2.853549
H	0.521084	2.655444	2.717401
H	-1.170493	2.548444	3.355275
H	-0.073851	1.140075	3.459970
C	0.980053	-1.135762	2.600321
C	0.447207	-1.661865	3.943095
C	-0.203739	-3.053999	3.883760

C	-1.647095	-3.085504	3.360573
C	-1.889966	-2.375927	2.021717
C	-0.954110	-2.700100	0.881665
H	-1.454899	-2.955577	-0.062294
H	-0.184982	-3.442211	1.127751
H	-2.949249	-2.455666	1.727909
H	-1.845628	-1.248299	2.278603
H	-2.316079	-2.639416	4.117608
H	-1.968340	-4.134763	3.245415
H	0.434528	-3.717248	3.273874
H	-0.211368	-3.498030	4.893014
H	1.281297	-1.710420	4.669066
H	-0.274975	-0.948506	4.389503
H	1.534737	-0.191649	2.754397
H	1.715725	-1.854954	2.196093
C	4.755392	0.783061	-3.042198
H	4.809751	0.345582	-4.054024
H	5.697336	0.581977	-2.503805
H	4.616514	1.868958	-3.127830

^{4}TS5-6B
Geometry with 79 atoms:
Total energy: -3196.974282870

Cr	0.027293	-0.044801	1.210840
P	-1.428973	0.309671	-0.800375
P	1.657058	0.000604	-0.635624
O	-0.103361	2.509331	0.673741
O	0.191757	-2.508496	-0.070715
C	0.910800	0.643105	-2.222802
C	-0.484624	0.034975	-2.384974
H	0.840908	1.739323	-2.149570
H	1.565375	0.402426	-3.074286
H	-1.030394	0.480149	-3.230861
H	-0.413411	-1.049140	-2.562143
C	-1.839517	2.097309	-0.890770
C	-2.839013	2.586285	-1.746389
C	-1.105625	3.017073	-0.104695
C	-3.132244	3.949397	-1.811900
H	-3.405144	1.884161	-2.363219
C	-1.404935	4.385614	-0.160568
C	-2.415400	4.841508	-1.011195
H	-3.916368	4.310735	-2.480296
H	-0.854989	5.101259	0.449270
H	-2.638005	5.910806	-1.046010
C	-3.008143	-0.597019	-0.995336
C	-3.016645	-1.859435	-1.617803
C	-4.197920	-0.119536	-0.413880
C	-4.188670	-2.618500	-1.665329
H	-2.109423	-2.263658	-2.070850
C	-5.365676	-0.885255	-0.459931
H	-4.221982	0.860346	0.067060
C	-5.365372	-2.135644	-1.085022
H	-4.180925	-3.592377	-2.161175
H	-6.281560	-0.498164	-0.006866
H	-6.280888	-2.730846	-1.122913
C	2.167471	-1.698737	-1.104171
C	3.332291	-1.943325	-1.847723
C	1.344117	-2.793006	-0.745902
C	3.700207	-3.240027	-2.211386
H	3.968284	-1.103801	-2.137930
C	1.718041	-4.097366	-1.101195
C	2.891463	-4.311972	-1.828911
H	4.612795	-3.410362	-2.786205
H	1.100276	-4.949472	-0.820408
H	3.169038	-5.333523	-2.100062
C	3.192611	0.967625	-0.391350
C	3.218535	2.338801	-0.703906
C	4.309955	0.393467	0.242854
C	4.343250	3.112530	-0.402973
H	2.362203	2.818358	-1.181984
C	5.431660	1.170820	0.540148
H	4.307828	-0.666778	0.503362
C	5.452380	2.531707	0.218344
H	4.351298	4.175102	-0.658451
H	6.294014	0.708623	1.026821
H	6.331500	3.137370	0.451316
C	0.611542	3.361953	1.564074
H	1.346499	2.726454	2.074650
H	1.148779	4.154871	1.019467
H	-0.063840	3.812522	2.310064
C	-0.669656	-3.568250	0.330358
H	-0.166765	-4.247732	1.038059
H	-1.527893	-3.098021	0.823949
H	-1.032597	-4.143464	-0.536853
C	1.720363	-0.736247	2.280545
C	0.666948	-0.586863	3.259142
C	-0.076999	-1.810308	3.807324
C	-1.510639	-1.490333	4.262773
C	-2.421941	-0.971449	3.134473
C	-1.894937	0.298412	2.449031
H	1.998495	-1.750439	1.968153
H	2.567392	-0.044613	2.334237
H	0.833482	0.191379	4.021760
H	-0.463224	0.031032	2.781968
H	-0.104977	-2.592137	3.027432
H	0.501076	-2.235191	4.646165
H	-1.469112	-0.733808	5.068315
H	-1.959352	-2.391220	4.712410
H	-2.548834	-1.768392	2.378545
H	-3.432622	-0.791946	3.544151
H	-2.565469	0.622256	1.645521
H	-1.857004	1.138468	3.167283

^{6}6B
Geometry with 79 atoms:
Total energy: -3197.040136790

Cr	-0.020085	-0.308864	-1.209492
P	-0.835691	1.118975	0.723687
P	2.119322	-0.362580	0.142763
O	-0.782189	-1.779477	1.007709
O	1.617003	2.160955	-1.231311
C	1.609765	0.217722	1.845857
C	0.660931	1.423433	1.797659
H	1.120820	-0.643156	2.327952
H	2.506069	0.473000	2.432309
H	0.342483	1.692932	2.816731
H	1.171670	2.295836	1.360276
C	-1.965476	0.116954	1.777020
C	-3.004687	0.675025	2.534302
C	-1.802791	-1.289509	1.776676
C	-3.864072	-0.133557	3.284135
H	-3.148745	1.757925	2.532891
C	-2.659001	-2.102327	2.528490
C	-3.685492	-1.517547	3.278354
H	-4.668363	0.318475	3.868350
H	-2.538410	-3.185163	2.535255
H	-4.350699	-2.159732	3.860760
C	-1.651391	2.749511	0.566431
C	-1.350525	3.854245	1.380331
C	-2.608516	2.893595	-0.455119
C	-1.992201	5.079489	1.170067
H	-0.618129	3.772724	2.185708
C	-3.256418	4.114012	-0.654236
H	-2.847309	2.043356	-1.100834
C	-2.944946	5.211707	0.156062
H	-1.747650	5.933463	1.806677
H	-4.001206	4.211399	-1.448027
H	-3.445036	6.170034	-0.004060
C	3.391524	0.863468	-0.367384
C	4.762043	0.676496	-0.141792
C	2.961284	2.038614	-1.029712
C	5.696032	1.632556	-0.551079
H	5.104967	-0.232671	0.357554
C	3.894693	3.000262	-1.437440
C	5.256289	2.790424	-1.194663
H	6.760330	1.470812	-0.367406
H	3.572313	3.909304	-1.944822
H	5.976654	3.545457	-1.518969
C	3.032311	-1.922551	0.436093
C	3.529465	-2.315167	1.690305
C	3.201912	-2.781218	-0.665871
C	4.179381	-3.545137	1.836607
H	3.417353	-1.668717	2.562599
C	3.861324	-4.003151	-0.518942
H	2.811055	-2.490401	-1.645669
C	4.347343	-4.389282	0.735193
H	4.559790	-3.842181	2.817132
H	3.990475	-4.658962	-1.383445
H	4.856530	-5.348887	0.853689
C	-0.486984	-3.171565	1.015137
H	0.373550	-3.307070	0.347254
H	-0.212327	-3.514949	2.026300
H	-1.335656	-3.768257	0.641291
C	1.088231	3.332089	-1.839168
H	1.475205	3.466226	-2.863415
H	0.000452	3.191279	-1.878715
H	1.309361	4.231582	-1.240206
C	-0.534485	-1.608417	-3.068169
C	-6.268441	-3.237295	-2.550150
C	-1.700105	-1.000224	-2.665214
H	0.082498	-1.184236	-3.867576
H	-0.298204	-2.632926	-2.756687
C	-5.049463	-2.779885	-1.750677
H	-5.987770	-3.972382	-3.323264
H	-6.752550	-2.388774	-3.062676
C	-2.752582	-1.657207	-1.804258
H	-1.995278	-0.061980	-3.155869
C	-3.974281	-2.119791	-2.617770
H	-4.606591	-3.643443	-1.221301
H	-5.364109	-2.072584	-0.961687
H	-2.316815	-2.522849	-1.276988
H	-3.098666	-0.959361	-1.021328
H	-3.640490	-2.822590	-3.401775
H	-4.408505	-1.253422	-3.149259
H	-7.023999	-3.708746	-1.901329

^{4}TS3-7B
Geometry with 73 atoms:
Total energy: -3118.348941130

Cr	0.087877	-0.323871	1.401516
P	-1.591368	0.214606	-0.449048
P	1.660212	-0.152118	-0.455387
O	-0.063360	2.708974	-0.400039
O	0.097767	-2.439971	0.424134
C	0.789703	0.306809	-2.036537
C	-0.663690	-0.187065	-2.024731
H	0.830606	1.400227	-2.119010
H	1.326858	-0.128619	-2.893175
H	-1.210718	0.209488	-2.893444
H	-0.683600	-1.287093	-2.091881
C	-2.264803	1.913461	-0.630237
C	-3.634961	2.162427	-0.799066
C	-1.379035	3.013349	-0.527242
C	-4.128166	3.468989	-0.856681
H	-4.330890	1.325645	-0.880812
C	-1.874175	4.323584	-0.573046
C	-3.245220	4.542863	-0.737632
H	-5.198020	3.642321	-0.989930
H	-1.199145	5.174410	-0.485542
H	-3.619787	5.568804	-0.774205
C	-3.075998	-0.861421	-0.510071
C	-3.505751	-1.530823	-1.667666
C	-3.805428	-1.024924	0.682893
C	-4.634152	-2.356966	-1.626693
H	-2.974573	-1.413227	-2.613657
C	-4.937461	-1.841200	0.717751
H	-3.488191	-0.507681	1.591751
C	-5.350544	-2.514710	-0.437196
H	-4.957059	-2.874605	-2.533371
H	-5.495737	-1.955413	1.650116
H	-6.232315	-3.159530	-0.410149
C	2.121891	-1.909994	-0.709521
C	3.300227	-2.312558	-1.350240
C	1.239651	-2.893278	-0.215806
C	3.598752	-3.668024	-1.511674
H	3.995411	-1.553999	-1.718669
C	1.530010	-4.251225	-0.375435
C	2.710858	-4.628641	-1.025170
H	4.521524	-3.970157	-2.011219
H	0.859838	-5.021041	0.004497
H	2.934527	-5.691733	-1.141954
C	3.209764	0.801039	-0.411836
C	3.775581	1.384731	-1.558731
C	3.836973	0.971437	0.835055
C	4.953451	2.130403	-1.454396
H	3.305119	1.264854	-2.536777
C	5.016856	1.711766	0.931376
H	3.392769	0.525892	1.728586
C	5.573916	2.294910	-0.211897
H	5.388408	2.583548	-2.348518
H	5.499065	1.840385	1.903389
H	6.493474	2.880112	-0.134307
C	0.891420	3.742237	-0.208264

H	1.865147	3.248220	-0.103209
H	0.926486	4.422809	-1.076215
H	0.679144	4.321054	0.705610
C	-0.921237	-3.388791	0.771904
H	-0.571370	-4.064185	1.568218
H	-1.777744	-2.809187	1.129878
H	-1.226365	-3.967890	-0.113119
C	0.369250	1.480899	2.367564
C	0.649314	0.909298	3.769302
H	1.215457	2.049965	1.960806
H	-0.541485	2.098059	2.308880
H	0.078086	1.406349	4.574658
H	1.715412	0.984340	4.031083
C	0.241666	-0.558979	3.703911
C	-1.039368	-0.857473	3.248446
H	1.339121	-0.848734	2.343210
H	0.833869	-1.315569	4.228459
H	-1.773678	-0.050828	3.154878
H	-1.432380	-1.876205	3.311915

^{4}7B

Geometry with 73 atoms:

Total energy: -3118.356005120

Cr	-0.144455	0.295960	1.423865
P	1.537119	-0.235577	-0.503319
P	-1.674293	0.183600	-0.427726
O	-0.021528	-2.705633	-0.418932
O	-0.014332	2.406066	0.470829
C	-0.864920	-0.287350	-2.036412
C	0.586767	0.204772	-2.052668
H	-0.915749	-1.380067	-2.122947
H	-1.423446	0.157230	-2.874542
H	1.120982	-0.171130	-2.938372
H	0.595441	1.305131	-2.098281
C	2.179315	-1.940284	-0.749727
C	3.531790	-2.210477	-1.006972
C	1.281317	-3.027938	-0.615550
C	3.998466	-3.523785	-1.111147
H	4.236035	-1.384848	-1.122583
C	1.751232	-4.345362	-0.705421
C	3.106312	-4.584909	-0.951963
H	5.054995	-3.712379	-1.312660
H	1.067448	-5.185954	-0.591546
H	3.460744	-5.616173	-1.023327
C	3.028301	0.834578	-0.562948
C	3.301412	1.735853	-1.605008
C	3.901368	0.792366	0.541547
C	4.413968	2.582127	-1.536104
H	2.657288	1.790493	-2.483446
C	5.016154	1.629673	0.603000
H	3.716977	0.088836	1.356359
C	5.271140	2.534155	-0.434229
H	4.612525	3.278088	-2.354912
H	5.687107	1.577533	1.463996
H	6.139580	3.195441	-0.384964
C	-2.061653	1.962883	-0.657932
C	-3.222389	2.415458	-1.296838
C	-1.141707	2.907704	-0.157691
C	-3.468878	3.782758	-1.446633
H	-3.946334	1.687274	-1.671251
C	-1.381235	4.276871	-0.303237
C	-2.546551	4.704680	-0.949599
H	-4.379314	4.124071	-1.943503
H	-0.682333	5.016268	0.085251
H	-2.730864	5.776445	-1.055221
C	-3.256142	-0.715871	-0.353389
C	-3.859000	-1.261744	-1.501087
C	-3.872131	-0.883674	0.899665
C	-5.061958	-1.965110	-1.392011
H	-3.400272	-1.145866	-2.485013
C	-5.075613	-1.584738	0.999887
H	-3.401465	-0.466490	1.792388
C	-5.670510	-2.128102	-0.143643
H	-5.525451	-2.386290	-2.287428
H	-5.548186	-1.711521	1.976895
H	-6.609860	-2.680475	-0.061975
C	-0.984228	-3.722718	-0.184889
H	-1.941997	-3.211160	-0.028173
H	-1.075063	-4.397127	-1.053736
H	-0.737282	-4.310684	0.714357
C	1.004110	3.318847	0.903398
H	0.637283	3.948608	1.729054
H	1.845623	2.708253	1.246744
H	1.342811	3.946442	0.065592
C	-0.382051	-1.515676	2.351414
C	-0.367238	-1.053144	3.817858
H	-1.309747	-2.034673	2.075849
H	0.476451	-2.156094	2.091723
H	0.170715	-1.751056	4.487985
H	-1.390012	-0.962160	4.210607
C	0.302442	0.309408	3.885988
C	1.490194	0.573961	3.288994
H	-1.523439	0.805527	2.122460
H	-0.203947	1.113681	4.431702
H	2.079926	-0.228891	2.833832
H	1.965757	1.555600	3.366880

^{4}TS7-8B

Geometry with 73 atoms:

Total energy: -3118.339152210

Cr	0.066076	-0.096667	1.405311
P	-1.568717	0.178368	-0.475197
P	1.566323	-0.171013	-0.470136
O	-0.001921	2.412143	0.676803
O	0.050088	-2.616616	0.118899
C	0.707063	0.301453	-2.064737
C	-0.707317	-0.282877	-2.066466
H	0.662164	1.401729	-2.106598
H	1.284280	-0.048652	-2.934057
H	-1.294448	0.075628	-2.926002
H	-0.665479	-1.381683	-2.111601
C	-1.879910	1.978343	-0.706560
C	-2.921389	2.452276	-1.519389
C	-1.013394	2.914254	-0.094956
C	-3.114571	3.819772	-1.722970
H	-3.596405	1.736909	-1.995362
C	-1.203777	4.288247	-0.299153
C	-2.252600	4.731235	-1.109266
H	-3.931898	4.169545	-2.356989
H	-0.544164	5.017537	0.169276
H	-2.392386	5.804757	-1.258280
C	-3.224445	-0.602608	-0.575430
C	-3.449637	-1.766403	-1.330814
C	-4.276998	-0.082444	0.202032
C	-4.700629	-2.392391	-1.310018
H	-2.656514	-2.196084	-1.944990
C	-5.524542	-0.708281	0.216979
H	-4.124487	0.825409	0.790850
C	-5.739524	-1.866993	-0.537815
H	-4.862841	-3.293232	-1.907039
H	-6.333637	-0.287569	0.819075
H	-6.716526	-2.355952	-0.526052
C	2.110400	-1.900027	-0.789185
C	3.350254	-2.197781	-1.370732
C	1.249516	-2.964743	-0.433978
C	3.739851	-3.520594	-1.598943
H	4.024511	-1.382247	-1.642389
C	1.638255	-4.291761	-0.656886
C	2.881652	-4.560510	-1.238629
H	4.709824	-3.734620	-2.052607
H	0.984628	-5.118998	-0.380809
H	3.176243	-5.599217	-1.407467
C	3.107196	0.821031	-0.435323
C	3.458471	1.724105	-1.452598
C	3.948102	0.697550	0.686724
C	4.622106	2.493856	-1.343041
H	2.835924	1.839021	-2.341060
C	5.112528	1.459870	0.787720
H	3.688907	-0.002188	1.484966
C	5.449774	2.365221	-0.225138
H	4.882870	3.193143	-2.141305
H	5.758473	1.349269	1.662201
H	6.358660	2.966288	-0.143355
C	1.024996	3.282114	1.153778
H	1.779270	2.641226	1.624906
H	1.494443	3.831192	0.321985
H	0.632904	3.994116	1.898338
C	-0.889719	-3.621390	0.472013
H	-0.496702	-4.285726	1.260078
H	-1.778455	-3.097515	0.845487
H	-1.180363	-4.226839	-0.402880
C	0.878475	0.415958	3.305481
C	0.168152	-0.576000	4.227765
H	1.914538	0.634037	3.599294
H	0.327294	1.377500	3.259535
H	-0.232739	-0.104592	5.143104
H	0.858981	-1.369161	4.548728
C	-0.934082	-1.179910	3.378512
C	-1.991204	-0.482515	2.899305
H	1.541097	-0.369572	1.952210
H	-0.837286	-2.237232	3.100738
H	-2.182924	0.553028	3.204422
H	-2.761321	-0.962134	2.290848

^{6}8B

Geometry with 73 atoms:

Total energy: -3118.425391550

Cr	0.006414	-0.209663	1.410936
P	-1.830670	0.189052	-0.284770
P	1.503332	0.206511	-0.604848
O	-0.404863	2.524578	0.711760
O	0.256071	-2.408398	-0.286885
C	0.372590	0.845631	-1.947089
C	-0.986951	0.134119	-1.951705
H	0.247088	1.922556	-1.753856
H	0.857840	0.732222	-2.928879
H	-1.641310	0.583957	-2.714463
H	-0.864367	-0.932706	-2.197018
C	-2.497717	1.901128	-0.192089
C	-3.797975	2.239718	-0.590708
C	-1.656705	2.915366	0.325388
C	-4.261901	3.554802	-0.492160
H	-4.460074	1.462963	-0.980455
C	-2.116682	4.234680	0.421704
C	-3.417461	4.545413	0.011272
H	-5.278206	3.800824	-0.806982
H	-1.475021	5.021679	0.817338
H	-3.768669	5.577008	0.092717
C	-3.294989	-0.894337	-0.463250
C	-3.810247	-1.315974	-1.700690
C	-3.910182	-1.338838	0.721597
C	-4.918391	-2.168133	-1.747992
H	-3.357967	-0.983473	-2.636777
C	-5.023530	-2.179799	0.670660
H	-3.511107	-1.023202	1.690396
C	-5.526955	-2.599401	-0.565793
H	-5.310240	-2.491981	-2.715421
H	-5.496460	-2.513777	1.597480
H	-6.393658	-3.263689	-0.607038
C	2.135293	-1.382497	-1.287105
C	3.319207	-1.478874	-2.030904
C	1.395280	-2.560917	-1.027426
C	3.764154	-2.710441	-2.520138
H	3.903973	-0.577176	-2.227308
C	1.835863	-3.795973	-1.517951
C	3.018482	-3.861889	-2.262580
H	4.688569	-2.767078	-3.098732
H	1.270345	-4.707097	-1.323585
H	3.355590	-4.830137	-2.640725
C	2.943175	1.337093	-0.620685
C	3.222651	2.231040	-1.667732
C	3.790503	1.313013	0.502236
C	4.328211	3.084619	-1.588512
H	2.587082	2.267604	-2.554405
C	4.899971	2.157349	0.573268
H	3.577159	0.628572	1.328252
C	5.167990	3.048774	-0.471695
H	4.535716	3.777907	-2.407385
H	5.553397	2.125155	1.448669
H	6.031434	3.716081	-0.414377
C	0.539868	3.496029	1.145676
H	1.466320	2.949575	1.363400
H	0.741963	4.238417	0.355411
H	0.198828	4.012304	2.058803
C	-0.602820	-3.517790	-0.053416
H	-0.096190	-4.308426	0.525157
H	-1.450964	-3.129459	0.525542
H	-0.980518	-3.937564	-1.000568
C	-0.347673	-0.832410	3.601649
C	1.018174	-0.829812	3.440524
H	-0.874337	0.033379	4.017749
H	-0.919791	-1.765535	3.529436
H	1.576348	0.075138	3.719532

C	1.846101	-2.069850	3.192165
H	1.215399	-2.853594	2.737878
H	2.646769	-1.851964	2.464264
C	2.479658	-2.602266	4.486854
H	1.705368	-2.878128	5.220434
H	3.094244	-3.493858	4.283470
H	3.129947	-1.844910	4.954593

^{4}9B

Geometry with 85 atoms:

Total energy: -3275.580967480

Cr	-0.674945	-0.532538	1.215044
P	-1.546330	0.306348	-0.900906
P	1.621560	-0.262681	-0.265892
O	-0.327767	1.870227	1.310532
O	4.037331	-0.354094	-2.021935
C	1.047598	0.385078	-1.926912
C	-0.361654	-0.102125	-2.271303
H	1.771826	0.081343	-2.693924
H	1.068361	1.483603	-1.887687
H	-0.717628	0.353381	-3.208998
H	-0.379162	-1.195920	-2.404318
C	-1.454944	2.130605	-0.773823
C	-1.961209	2.962456	-1.784953
C	-1.860976	4.350461	-1.691961
C	-1.248243	4.916108	-0.570915
C	-0.736941	4.110999	0.450111
C	-0.835683	2.715952	0.350949
H	-0.262160	4.579614	1.310467
H	-1.164391	6.001817	-0.481140
H	-2.261411	4.985194	-2.484927
H	-2.452144	2.510926	-2.650706
C	-3.213713	-0.063915	-1.540931
C	-3.409407	-1.060142	-2.513095
C	-4.701984	-1.391397	-2.928332
C	-5.807513	-0.737210	-2.377899
C	-5.618609	0.257620	-1.412742
C	-4.330113	0.594222	-0.993997
H	-4.195377	1.377021	-0.244240
H	-6.478908	0.775958	-0.982655
H	-6.817145	-0.999899	-2.702767
H	-4.843096	-2.167056	-3.684854
H	-2.562151	-1.593385	-2.947885
C	2.668453	-1.713210	-0.671744
C	2.375723	-2.971315	-0.125136
C	3.172834	-4.087009	-0.396093
C	4.285472	-3.944008	-1.225765
C	4.605411	-2.703677	-1.786363
C	3.802393	-1.585016	-1.518278
H	5.478407	-2.617258	-2.432929
H	4.919427	-4.806435	-1.446876
H	2.923778	-5.056827	0.039200
H	1.503750	-3.084029	0.517868
C	2.818282	0.989100	0.360965
C	2.633334	2.365836	0.152927
C	3.506904	3.295158	0.726406
C	4.572761	2.865957	1.522420
C	4.763616	1.496961	1.736502
C	3.895391	0.566169	1.160939
H	4.069641	-0.500103	1.324520
H	5.598542	1.148808	2.349894
H	5.255267	3.593333	1.968524
H	3.351576	4.361835	0.544474
H	1.808399	2.736128	-0.457586
C	1.313400	-1.081768	2.968810
C	0.153847	-1.239635	3.631960
H	-0.356358	-2.205075	3.666256
H	-0.285253	-0.435952	4.229463
H	1.790422	-1.916600	2.448424
H	1.875325	-0.142751	2.989324
C	-1.068840	-2.480983	0.684184
C	-2.473509	-3.056114	0.491903
C	-3.318528	-3.284436	1.752799
C	-4.048293	-2.072953	2.348597
C	-3.205491	-1.051544	3.121806
C	-2.389671	-0.067048	2.282952
H	-2.000256	0.736734	2.938062
H	-3.068648	0.437941	1.571667
H	-2.561644	-1.594681	3.837200
H	-3.900492	-0.467068	3.756668
H	-4.816406	-2.461517	3.040005
H	-4.604806	-1.554430	1.545246
H	-4.088750	-4.033494	1.499424
H	-2.694570	-3.759010	2.534612
H	-3.053804	-2.435620	-0.211342
H	-2.368395	-4.036495	-0.013287
H	-0.496723	-2.606680	-0.254100
H	-0.528779	-3.068276	1.454268
C	0.145951	2.438992	2.537401
H	0.412682	1.602812	3.190712
H	1.041480	3.054096	2.365060
H	-0.643786	3.033332	3.021837
C	5.213493	-0.097551	-2.772992
H	5.227610	-0.669318	-3.717014
H	5.200474	0.975930	-3.003596
H	6.121729	-0.328801	-2.190578

^{4}TS9-10B

Geometry with 85 atoms:

Total energy: -3275.563472970

Cr	-0.534934	-0.689184	1.055591
P	1.576358	-0.304888	-0.351180
P	-1.489834	0.393053	-0.987335
O	4.099910	-0.166601	-1.878912
O	-0.337506	1.689048	1.433078
C	-0.346474	0.048023	-2.405225
C	1.093030	0.406809	-2.018623
H	-0.436761	-1.026977	-2.630832
H	-0.663269	0.605755	-3.300805
H	1.806244	0.046312	-2.771213
H	1.209063	1.498377	-1.974899
C	2.707010	-1.689670	-0.749791
C	2.431105	-2.997340	-0.327015
C	3.900776	-1.441314	-1.478027
C	3.311358	-4.047501	-0.603533
H	1.512983	-3.201129	0.221712
C	4.788477	-2.493094	-1.745612
C	4.487404	-3.786641	-1.308003
H	3.078345	-5.059476	-0.266407
H	5.710291	-2.311935	-2.298419
H	5.186712	-4.597610	-1.526676
C	2.669485	0.941367	0.451231
C	2.571821	2.318024	0.198707
C	3.577017	0.493445	1.427700
C	3.370294	3.226588	0.900716
H	1.870493	2.705855	-0.540670
C	4.371750	1.403018	2.129088
H	3.674653	-0.574705	1.635597
C	4.271965	2.773977	1.868153
H	3.284020	4.294893	0.686101
H	5.076677	1.037002	2.879744
H	4.897369	3.484917	2.413567
C	-1.313371	2.190795	-0.689880
C	-1.725052	3.134999	-1.644060
C	-0.740342	2.640425	0.519152
C	-1.570314	4.502205	-1.418234
H	-2.183928	2.784777	-2.572513
C	-0.585484	4.014993	0.750926
C	-0.999253	4.932744	-0.217467
H	-1.896220	5.225193	-2.168669
H	-0.137382	4.381744	1.672470
H	-0.871811	6.000473	-0.023106
C	-3.193578	0.167867	-1.595375
C	-4.249627	0.727405	-0.851760
C	-3.486437	-0.646754	-2.702028
C	-5.574436	0.476010	-1.212412
H	-4.036664	1.368032	0.007913
C	-4.815617	-0.894662	-3.057565
H	-2.686683	-1.099468	-3.291342
C	-5.860124	-0.338016	-2.314304
H	-6.387286	0.917519	-0.630781
H	-5.034135	-1.527540	-3.921114
H	-6.897601	-0.535823	-2.594239
C	5.334069	0.216784	-2.463825
H	5.272884	1.301547	-2.623507
H	6.182254	-0.000710	-1.792442
H	5.498189	-0.281397	-3.434995
C	0.155207	2.137049	2.703754
H	1.093537	2.697005	2.581581
H	-0.598833	2.754618	3.215501
H	0.351977	1.242583	3.301299
C	-2.237310	-0.504163	2.464875
C	-3.319449	-1.358546	3.110101
C	-4.058539	-2.320990	2.173967
C	-3.243822	-3.418791	1.469104
C	-2.492800	-3.028569	0.179197
C	-1.043288	-2.550251	0.315669
H	-2.069852	0.430719	3.016593
H	-2.598710	-0.222508	1.456022
H	-2.920888	-1.919506	3.975139
H	-4.072589	-0.675105	3.543962
H	-4.845101	-2.810526	2.773417
H	-4.594498	-1.734745	1.404717
H	-3.958385	-4.213765	1.198245
H	-2.544178	-3.890370	2.183948
H	-2.479498	-3.925239	-0.470083
H	-3.098591	-2.291675	-0.376420
H	-0.483260	-3.269022	0.942821
H	-0.562968	-2.573128	-0.680412
C	0.763634	-1.350491	2.631441
C	-0.487794	-1.515179	3.259518
H	1.433558	-0.552153	2.966363
H	1.267762	-2.229358	2.222392
H	-0.948231	-2.504728	3.243944
H	-0.726127	-0.933687	4.153338

^{4}10B

Geometry with 85 atoms:

Total energy: -3275.605705410

Cr	-0.391543	-0.432296	0.918641
P	-1.905247	-0.004855	-0.893382
P	1.375008	0.324198	-0.932614
O	-0.756297	1.927995	0.994519
O	3.526869	-1.020415	0.393976
C	0.289899	0.892033	-2.342538
C	-0.976055	0.037688	-2.498406
H	0.851947	0.923165	-3.287975
H	0.018837	1.933444	-2.106381
H	-0.726324	-1.001513	-2.762891
H	-1.629656	0.436800	-3.290269
C	-2.458597	1.720586	-0.659208
C	-3.493119	2.288925	-1.417942
C	-3.854572	3.626032	-1.248609
C	-3.169865	4.405159	-0.313037
C	-2.132584	3.864655	0.452262
C	-1.775267	2.521127	0.282304
H	-1.616811	4.498555	1.171750
H	-3.441227	5.453845	-0.169853
H	-4.663735	4.056327	-1.841970
H	-4.025728	1.668901	-2.143623
C	-3.380168	-1.043583	-1.124506
C	-3.298582	-2.217075	-1.895620
C	-4.400503	-3.070047	-1.992193
C	-5.585988	-2.767748	-1.315399
C	-5.667497	-1.608996	-0.536789
C	-4.570879	-0.750407	-0.435642
H	-4.647402	0.150615	0.175849
H	-6.590440	-1.369840	-0.003003
H	-6.446127	-3.437104	-1.392734
H	-4.330039	-3.976373	-2.598256
H	-2.377687	-2.478666	-2.420789
C	2.420459	-0.993388	-1.671877
C	2.243614	-1.509029	-2.962530
C	3.034273	-2.562523	-3.433559
C	4.016691	-3.108638	-2.607188
C	4.216173	-2.612950	-1.314843
C	3.420158	-1.560551	-0.846621
H	4.985709	-3.052808	-0.680746
H	4.639676	-3.931940	-2.965020
H	2.881709	-2.949908	-4.443059
H	1.483341	-1.091515	-3.624584
C	2.512729	1.748966	-0.666875
C	3.053218	1.952349	0.614108
C	3.914719	3.023264	0.861819
C	4.245520	3.908294	-0.169442
C	3.716060	3.712910	-1.448552
C	2.857963	2.637782	-1.698664
H	2.468108	2.496839	-2.708643
H	3.976333	4.397251	-2.259802
H	4.918475	4.747514	0.023049
H	4.330341	3.166594	1.862517
H	2.810358	1.257642	1.419940
C	4.559503	-1.444911	1.266883

H	4.495514	-0.808252	2.159336
H	5.554578	-1.312500	0.809118
H	4.430813	-2.499217	1.566847
C	-0.191381	-2.406304	0.361868
C	0.868066	-3.142510	1.192861
C	0.723310	-2.883238	2.695983
C	1.163837	-1.477385	3.118526
C	0.644419	-0.997536	4.474306
H	1.069317	-1.661496	5.247876
H	1.059398	0.005727	4.681198
C	-0.881074	-0.955120	4.651811
C	-1.668151	-0.033519	3.704418
C	-1.950432	-0.555685	2.284078
H	-2.331053	-1.591622	2.319756
H	-2.760850	0.054674	1.844886
H	-2.639528	0.170806	4.194312
H	-1.168498	0.954075	3.670833
H	-1.071685	-0.628745	5.688194
H	-1.296763	-1.975111	4.585423
H	0.918047	-0.694629	2.350200
H	2.264818	-1.423461	3.099586
H	1.324000	-3.605584	3.275216
H	-0.325501	-3.055776	2.984208
H	1.879300	-2.845923	0.871425
H	0.800371	-4.230777	1.005821
H	-1.186608	-2.858251	0.517804
H	0.045308	-2.486677	-0.714386
C	-0.004099	2.725889	1.915344
H	0.520199	3.537867	1.389389
H	-0.652505	3.134345	2.705365
H	0.736921	2.059927	2.369487

^{4}10B'

Geometry with 85 atoms:

Total energy: -3275.604883010

Cr	-0.042811	-0.176133	0.977089
P	1.632241	0.278730	-0.821504
P	-1.713961	0.399035	-0.854122
O	3.033311	-1.871026	0.455582
O	-0.281805	2.290285	0.893906
C	-0.696535	0.517449	-2.408613
C	0.658868	1.182132	-2.124963
H	-0.555365	-0.511101	-2.777410
H	-1.250258	1.079429	-3.177133
H	1.238097	1.284312	-3.054752
H	0.513253	2.200284	-1.731349
C	2.342930	-1.181304	-1.673801
C	2.249479	-1.402454	-3.054287
C	2.754217	-2.572000	-3.630526
C	3.359501	-3.532315	-2.818255
C	3.470490	-3.335024	-1.438746
C	2.968593	-2.160027	-0.863869
H	3.948800	-4.094651	-0.820908
H	3.755716	-4.450626	-3.258563
H	2.673452	-2.728768	-4.708083
H	1.777412	-0.661476	-3.701757
C	3.040467	1.389956	-0.425787
C	3.399844	2.469503	-1.250277
C	4.457776	3.309510	-0.888768
C	5.170692	3.076731	0.290677
C	4.823985	1.997518	1.110419
C	3.763124	1.160352	0.758999
H	3.490800	0.323220	1.400602
H	5.379922	1.808065	2.032052
H	5.997762	3.734208	0.569615
H	4.727583	4.147187	-1.536683
H	2.867295	2.667177	-2.182154
C	-2.203734	2.135378	-0.513080
C	-3.346948	2.721572	-1.076278
C	-3.703440	4.037211	-0.774535
C	-2.910532	4.776279	0.104823
C	-1.764306	4.216373	0.678006
C	-1.408116	2.898095	0.368652
H	-1.167196	4.814512	1.364566
H	-3.180903	5.804528	0.356729
H	-4.596775	4.479107	-1.220621
H	-3.970686	2.132738	-1.752802
C	-3.265627	-0.448140	-1.304287
C	-3.471663	-1.060470	-2.550014
C	-4.659147	-1.756582	-2.802179
C	-5.647846	-1.843562	-1.819883
C	-5.449495	-1.232399	-0.575823
C	-4.264332	-0.545385	-0.316241
H	-4.114994	-0.079703	0.662220
H	-6.219006	-1.297549	0.197185
H	-6.573573	-2.387981	-2.021289
H	-4.809400	-2.230621	-3.775208
H	-2.716467	-1.004659	-3.335465
C	0.688378	3.128577	1.539488
H	1.576993	2.515118	1.705943
H	0.308694	3.500750	2.503642
H	0.958458	3.974494	0.889233
C	3.536850	-2.826103	1.374182
H	2.956290	-3.763655	1.340030
H	4.601988	-3.045298	1.186015
H	3.435527	-2.379477	2.372044
C	0.986504	-0.036367	2.724114
C	-0.377277	0.148811	3.348930
C	-0.773079	-0.809361	4.485481
C	-0.890798	-2.265538	4.028964
C	-2.143682	-2.549757	3.175108
H	-2.956737	-2.876387	3.844556
H	-2.515678	-1.616653	2.713449
C	-1.929316	-3.586875	2.061898
C	-1.476252	-3.012162	0.711243
C	-0.156569	-2.227163	0.656013
H	0.618140	-2.682153	1.295640
H	0.232689	-2.272351	-0.375563
H	-1.399665	-3.863782	0.007524
H	-2.301402	-2.399005	0.309988
H	-2.871580	-4.133040	1.885305
H	-1.204721	-4.347047	2.407915
H	-0.895195	-2.927890	4.910165
H	0.016844	-2.537276	3.467860
H	-1.730028	-0.481396	4.928395
H	-0.011052	-0.715595	5.276850
H	-1.205958	0.010162	2.555297
H	-0.542409	1.196766	3.646773
H	1.485974	-0.980502	2.979640
H	1.670562	0.808478	2.868170

^{4}TS10-11B

Geometry with 85 atoms:

Total energy: -3275.591723150

Cr	-0.027823	0.100852	1.158811
P	-1.635756	0.276728	-0.740284
P	1.487104	0.271218	-0.888063
O	-0.429513	2.569862	0.705075
O	0.163438	-2.360461	-0.495928
C	0.518460	0.998082	-2.304695
C	-0.813056	0.256231	-2.413667
H	0.347410	2.064037	-2.087933
H	1.104613	0.929625	-3.233707
H	-1.475908	0.708396	-3.167203
H	-0.636633	-0.790709	-2.701401
C	-2.285555	1.998143	-0.661575
C	-3.450791	2.380561	-1.342881
C	-1.578971	2.975230	0.078512
C	-3.923318	3.693395	-1.288824
H	-4.002609	1.632902	-1.917656
C	-2.052894	4.292680	0.139564
C	-3.221329	4.642429	-0.543370
H	-4.833783	3.970768	-1.824075
H	-1.521498	5.051857	0.712176
H	-3.580879	5.672797	-0.488126
C	-3.113966	-0.792873	-0.926258
C	-3.136139	-1.851537	-1.851838
C	-4.223313	-0.614246	-0.077221
C	-4.236746	-2.711180	-1.921693
H	-2.298561	-2.022140	-2.529575
C	-5.320031	-1.474895	-0.150871
H	-4.241932	0.210959	0.635956
C	-5.329513	-2.528591	-1.070798
H	-4.238487	-3.525827	-2.650222
H	-6.173594	-1.317722	0.513014
H	-6.188723	-3.201279	-1.127138
C	2.017094	-1.353787	-1.572605
C	3.132652	-1.468050	-2.417365
C	1.271005	-2.519624	-1.271984
C	3.527835	-2.703017	-2.935006
H	3.708469	-0.574482	-2.667501
C	1.672457	-3.762555	-1.783414
C	2.797524	-3.846933	-2.607398
H	4.400718	-2.768828	-3.587651
H	1.113413	-4.666972	-1.546384
H	3.098551	-4.821836	-2.998720
C	3.011288	1.285572	-0.794864
C	2.985396	2.650004	-1.134644
C	4.192092	0.743262	-0.253320
C	4.118211	3.448191	-0.948686
H	2.083977	3.104116	-1.550523
C	5.321711	1.543725	-0.072113
H	4.232993	-0.311722	0.024570
C	5.288561	2.898370	-0.418566
H	4.084873	4.504715	-1.226151
H	6.232148	1.105110	0.343504
H	6.173636	3.523202	-0.276811
C	0.347454	3.509232	1.445364
H	1.219581	2.959777	1.819843
H	0.693300	4.334712	0.802617
H	-0.222234	3.915209	2.297407
C	-0.662921	-3.478981	-0.195681
H	-0.117083	-4.238808	0.385946
H	-1.496030	-3.091710	0.402736
H	-1.066457	-3.934907	-1.114032
C	1.932121	0.164842	2.357263
C	2.599849	-1.214818	2.328901
H	2.469065	0.890089	1.732420
H	2.009418	0.568457	3.384984
C	-1.850326	-0.009679	2.224080
C	1.993016	-2.248672	3.292142
H	2.579369	-1.632270	1.306210
H	3.671255	-1.098356	2.580643
C	-0.837820	0.219387	3.232804
H	-2.542851	0.811555	2.012656
H	-2.324130	-0.997225	2.169489
C	0.532178	-2.646455	2.975115
H	2.629264	-3.148274	3.271632
H	2.066787	-1.862712	4.324111
C	-0.592721	-0.766426	4.383971
H	0.448716	0.214452	2.760933
H	-0.808750	1.259088	3.597385
C	-0.525271	-2.253100	4.017948
H	0.466763	-3.737011	2.829885
H	0.253552	-2.222406	1.994898
H	0.335424	-0.474960	4.904781
H	-1.401302	-0.621946	5.121410
H	-1.513949	-2.590120	3.660840
H	-0.337102	-2.817938	4.947382

^{6}11B

Geometry with 85 atoms:

Total energy: -3275.653699000

Cr	0.266440	-0.215720	-1.200615
P	0.034545	1.462228	0.696962
P	2.343330	-0.892877	0.099308
O	-0.790996	-1.279514	1.230224
O	2.627070	1.606322	-1.374363
C	2.138740	-0.109511	1.784642
C	1.600002	1.325424	1.708408
H	1.440378	-0.755316	2.337224
H	3.103572	-0.117423	2.315373
H	1.423556	1.714890	2.722981
H	2.331460	1.985019	1.215707
C	-1.311040	0.940216	1.842434
C	-2.108206	1.848449	2.552397
C	-1.589263	-0.443268	1.958416
C	-3.155171	1.405539	3.366642
H	-1.911259	2.919030	2.462862
C	-2.634372	-0.891201	2.774454
C	-3.412210	0.038194	3.473858
H	-3.765857	2.128194	3.911959
H	-2.852528	-1.954808	2.867646
H	-4.228479	-0.319619	4.106104
C	-0.218325	3.262059	0.472435
C	0.412721	4.242290	1.256795
C	-1.083281	3.666787	-0.560897
C	0.183354	5.599302	1.007143
H	1.083337	3.960583	2.070626
C	-1.319799	5.021941	-0.800096
H	-1.573594	2.913436	-1.184601
C	-0.682545	5.991385	-0.017769
H	0.680668	6.353537	1.622100

H -1.997093 5.322830 -1.603116
H -0.860800 7.052642 -0.207872
C 3.919766 -0.175420 -0.517753
C 5.162400 -0.797293 -0.335935
C 3.865898 1.055911 -1.214673
C 6.337028 -0.214229 -0.820039
H 5.212513 -1.754296 0.188840
C 5.042218 1.645349 -1.695508
C 6.270170 1.006136 -1.493893
H 7.297146 -0.712310 -0.669437
H 5.013209 2.595766 -2.227751
H 7.181503 1.474179 -1.874164
C 2.710669 -2.654001 0.444774
C 3.118372 -3.137718 1.699273
C 2.531183 -3.564203 -0.613445
C 3.338563 -4.506002 1.888976
H 3.269574 -2.456212 2.538264
C 2.763043 -4.927978 -0.424129
H 2.203605 -3.200353 -1.592005
C 3.163390 -5.401710 0.830222
H 3.652589 -4.872186 2.869637
H 2.625032 -5.623954 -1.255301
H 3.338150 -6.469703 0.982103
C -0.933748 -2.689454 1.344323
H -0.191799 -3.126599 0.663790
H -0.724877 -3.029939 2.372379
H -1.941894 -3.022642 1.046063
C 2.481570 2.865937 -2.016812
H 2.845565 2.834296 -3.057778
H 1.406735 3.087522 -2.015475
H 3.009798 3.661957 -1.465278
C -9.148157 -1.758945 -1.318044
C -7.765746 -1.613976 -0.683086
H -9.431952 -0.847746 -1.871692
H -9.926768 -1.943241 -0.560225
C -0.753273 -1.454124 -2.877809
C -6.654107 -1.360374 -1.705179
H -7.778806 -0.787001 0.050290
H -7.525480 -2.525488 -0.105424
C -1.679958 -0.531981 -2.453120
H -0.130925 -1.271049 -3.760440
H -0.757535 -2.477327 -2.482976
C -5.265218 -1.214059 -1.080213
H -6.639215 -2.186233 -2.440470
H -6.892039 -0.448177 -2.283520
C -2.771513 -0.814155 -1.449665
H -9.173950 -2.598878 -2.033022
H -1.771478 0.410793 -3.010843
C -4.156651 -0.957812 -2.103898
H -5.024094 -2.127004 -0.504023
H -5.277362 -0.390023 -0.342921
H -2.534173 -1.734792 -0.891238
H -2.822774 -0.003263 -0.702198
H -4.126465 -1.779817 -2.840614
H -4.387498 -0.041761 -2.677123

^{4}5C
Geometry with 83 atoms:
Total energy: -3125.156408180
Cr 0.031949 -0.679998 1.183725
P -1.762183 0.085000 -0.311807
C -3.154280 -1.063212 -0.568676
C -3.523212 -1.560325 -1.828362
C -4.588651 -2.458426 -1.940555
C -5.290070 -2.864630 -0.801769
C -4.918687 -2.379633 0.457311
C -3.851076 -1.488677 0.576318
H -3.555947 -1.121582 1.562725
H -5.460399 -2.699728 1.350575
H -6.124662 -3.563772 -0.894197
H -4.872609 -2.839300 -2.924518
H -2.995744 -1.247068 -2.731508
C -2.387058 1.732770 0.213117
C -3.426676 2.464807 -0.411117
C -3.720198 3.743903 0.093450
C -3.022807 4.297645 1.167516
C -1.997240 3.573039 1.779916
C -1.692005 2.301134 1.300117
H -0.892706 1.730824 1.785033
H -1.442286 3.992527 2.621926
H -3.279779 5.297445 1.526030
H -4.519996 4.320494 -0.379815
C -4.271848 1.941154 -1.553714
C -5.634379 1.406200 -1.090468
H -6.220942 1.044272 -1.949513
H -5.514608 0.570138 -0.385612
H -6.218043 2.192894 -0.586581
H -3.747753 1.149314 -2.103018
H -4.430745 2.761147 -2.273649
C -0.938451 0.365206 -1.955693
C 0.312411 1.239191 -1.777413
P 1.532159 0.531623 -0.555289
C 2.592775 1.966497 -0.142923
C 2.579888 2.479569 1.163207
C 3.383129 3.572985 1.500188
C 4.203710 4.159507 0.532515
C 4.220756 3.653201 -0.772616
C 3.421109 2.559714 -1.110894
H 3.456014 2.155013 -2.125718
H 4.866326 4.108135 -1.527799
H 4.835683 5.011158 0.795925
H 3.372401 3.962942 2.520821
H 1.950684 2.017922 1.929893
C 2.600209 -0.636332 -1.492998
C 2.321303 -0.945228 -2.837021
C 3.066039 -1.904540 -3.524776
C 4.101572 -2.573563 -2.869139
C 4.383360 -2.273294 -1.536071
C 3.650447 -1.312293 -0.822057
C 4.046959 -1.026509 0.612513
C 5.295119 -0.141483 0.734036
H 6.162586 -0.619942 0.252459
H 5.548311 0.032256 1.792094
H 5.142130 0.836608 0.255210
H 4.234563 -1.985673 1.123545
H 3.212825 -0.555122 1.156739
H 5.193404 -2.801821 -1.025352
H 4.687915 -3.331791 -3.393842
H 2.833861 -2.128223 -4.568667
H 1.513527 -0.439614 -3.367554
H 0.797894 1.443260 -2.743882
H 0.035324 2.219984 -1.357846
H -0.681180 -0.630360 -2.351642
H -1.632110 0.837550 -2.667002
C -0.889039 -1.282520 2.883406
C 0.528398 -1.537046 3.331622
C 0.979217 -2.995094 3.503770
C 0.621987 -3.958119 2.361584
H -0.465816 -4.144932 2.349127
H 1.086315 -4.929609 2.597913
C 1.064058 -3.514722 0.957743
C 0.140601 -2.507923 0.272926
H -0.896236 -2.885168 0.235800
H 0.477379 -2.310288 -0.759642
H 1.119198 -4.414448 0.315319
H 2.099995 -3.130821 0.993475
H 0.534174 -3.370152 4.440957
H 2.072765 -3.004930 3.656012
H 0.807902 -0.947036 4.220577
H 1.279827 -1.074876 2.570825
H -1.532026 -2.167773 2.810691
H -1.398049 -0.466958 3.420760

^{4}9C
Geometry with 89 atoms:
Total energy: -3204.268681830
Cr 0.179857 -0.983650 1.265570
P -1.571689 0.241277 -0.291606
C -2.839460 -0.955691 -0.858784
C -2.587597 -1.812884 -1.943896
C -3.507443 -2.807186 -2.287358
C -4.685121 -2.961472 -1.549587
C -4.942066 -2.112303 -0.469016
C -4.026180 -1.115395 -0.122711
H -4.243818 -0.454653 0.719237
H -5.862580 -2.223614 0.109040
H -5.401858 -3.741169 -1.817594
H -3.301342 -3.464335 -3.135773
H -1.672083 -1.716924 -2.532088
C -2.492692 1.699478 0.347683
C -2.208828 2.058816 1.679757
C -2.785546 3.180753 2.272905
C -3.662830 3.968097 1.523763
C -3.965385 3.610509 0.209903
C -3.408465 2.475785 -0.406354
C -3.851390 2.152013 -1.820356
H -3.264103 1.325397 -2.235714
C -5.339494 1.789357 -1.922126
H -5.569160 0.893678 -1.325113
H -5.984703 2.607753 -1.566373
H -5.613180 1.577841 -2.967961
H -3.646882 3.028434 -2.459669
H -4.659889 4.229944 -0.364124
H -4.117832 4.858883 1.964008
H -2.551207 3.436319 3.308905
H -1.527712 1.440173 2.263463
C -0.692368 0.811948 -1.843638
C 0.647551 0.102878 -2.074107
P 1.732519 0.198205 -0.559673
C 3.308825 -0.612053 -1.047823
C 3.419672 -1.290692 -2.277258
C 4.582580 -1.984191 -2.615484
C 5.656346 -2.009616 -1.723091
C 5.555380 -1.340434 -0.503331
C 4.396370 -0.636844 -0.139020
C 4.375312 0.070611 1.201444
C 5.323774 1.273076 1.286417
H 6.366531 0.974469 1.095666
H 5.282966 1.728686 2.288646
H 5.053988 2.045392 0.551381
H 4.649891 -0.658476 1.983358
H 3.354830 0.404060 1.438794
H 6.396476 -1.365983 0.195155
H 6.570687 -2.552234 -1.975322
H 4.646971 -2.501318 -3.575760
H 2.598141 -1.284102 -2.994064
C 2.086030 2.002152 -0.488218
C 1.269800 2.826975 0.305071
C 1.472002 4.209857 0.332709
C 2.497836 4.781157 -0.425668
C 3.314434 3.967165 -1.218623
C 3.110311 2.585269 -1.254013
H 3.756333 1.959289 -1.874104
H 4.116613 4.410672 -1.813640
H 2.662149 5.861152 -0.400195
H 0.825415 4.838244 0.950102
H 0.460209 2.395888 0.896649
H 0.491894 -0.964723 -2.296627
H 1.166022 0.552327 -2.935807
H -1.343308 0.675331 -2.719042
H -0.539009 1.895662 -1.725323
C -1.363399 -1.827239 2.393664
C -1.521794 -3.352154 2.442538
H -0.677405 -3.818363 2.981586
C -1.695208 -4.031709 1.073539
C -0.411030 -4.258251 0.263335
C 0.495901 -3.026391 0.090413
C 1.384450 -2.645823 1.237009
H 1.308455 -3.288238 2.120873
H 2.428502 -2.445576 0.967649
H 1.065936 -3.071554 -0.852435
H -0.239687 -2.164071 -0.160544
H 0.193959 -5.053577 0.730043
H -0.692961 -4.629195 -0.735904
H -2.174344 -5.014998 1.213005
H -2.401934 -3.436300 0.470756
H -2.416505 -3.590222 3.048877
H -2.304603 -1.386930 2.020612
H -1.228186 -1.431347 3.416865
C 0.944378 0.429160 3.101284
C 1.523667 -0.762835 3.380894
H 1.018984 -1.513878 3.993103
H 2.556915 -0.977297 3.103338
H -0.033913 0.685644 3.517207
H 1.497369 1.227877 2.599180

^{4}TS5-6C
Geometry with 83 atoms:
Total energy: -3125.134852530
Cr -0.006356 -0.038947 1.288896
P 1.637597 0.414958 -0.532893
P -1.461080 -0.042152 -0.751939
C -0.537210 0.609368 -2.235589

C 0.888921 0.060602 -2.205637
H -1.061009 0.348380 -3.166296
H -0.537648 1.707499 -2.171838
H 0.890898 -1.030717 -2.341381
H 1.507584 0.482669 -3.011270
C 3.228613 -0.508152 -0.499451
C 3.211828 -1.914614 -0.328529
C 4.457572 0.173509 -0.556064
C 4.440540 -2.587979 -0.239554
C 5.665389 -0.519645 -0.467281
C 5.656466 -1.907442 -0.309787
H 4.438063 -3.672846 -0.100987
H 6.609984 0.027322 -0.513906
H 6.596175 -2.459736 -0.232172
C 2.037490 2.206722 -0.635645
C 1.738128 3.046634 0.450434
C 2.601638 2.772791 -1.794170
C 1.991916 4.419511 0.381960
H 1.296698 2.633194 1.359180
C 2.855213 4.144283 -1.861257
H 2.858621 2.144417 -2.649415
C 2.549471 4.970729 -0.774402
H 1.751501 5.058230 1.235235
H 3.295782 4.569394 -2.766294
H 2.747777 6.043850 -0.829944
C -3.067094 0.856108 -0.727948
C -3.106861 2.234220 -0.400504
C -4.263950 0.165104 -0.995050
C -4.356808 2.874806 -0.391650
C -5.493594 0.823277 -0.964095
C -5.538823 2.187510 -0.668450
H -4.397830 3.942220 -0.156123
H -6.411645 0.270216 -1.176184
H -6.494474 2.717144 -0.651290
C -1.837105 -1.780066 -1.234119
C -2.172302 -2.131697 -2.554444
C -1.780445 -2.791598 -0.260040
C -2.440159 -3.461394 -2.887507
H -2.239419 -1.369949 -3.333581
C -2.054950 -4.120883 -0.592854
H -1.522490 -2.546405 0.770260
C -2.384089 -4.458781 -1.908106
H -2.698239 -3.718740 -3.917635
H -2.008469 -4.892737 0.179148
H -2.596072 -5.497893 -2.171348
C 1.775124 -0.034266 2.436911
C 0.702019 -0.093913 3.399163
C 0.450352 -1.371869 4.208751
C -1.017165 -1.544221 4.623019
C -1.964101 -1.693804 3.421154
C -1.971165 -0.490403 2.461473
H 2.351070 -0.948834 2.249625
H 2.386446 0.872252 2.378184
H 0.542327 0.823113 3.989315
H -0.552747 -0.101301 2.839952
H 0.767411 -2.244388 3.608472
H 1.103130 -1.356158 5.097946
H -1.328906 -0.673932 5.229911
H -1.111760 -2.425438 5.277783
H -1.683118 -2.610904 2.870208
H -2.990714 -1.874203 3.787313
H -2.643997 -0.679412 1.615386
H -2.372709 0.401921 2.972999
H 4.478702 1.258750 -0.663344
H -4.239726 -0.899689 -1.232008
C 1.936358 -2.729521 -0.238364
C 1.686827 -3.629627 -1.454194
H 1.067242 -2.063439 -0.097747
H 1.978507 -3.355382 0.669751
H 0.737598 -4.176113 -1.347109
H 1.640198 -3.046263 -2.387291
H 2.494975 -4.367929 -1.572735
C -1.888258 3.053865 -0.017499
C -1.814671 3.364028 1.483260
H -1.908184 4.002533 -0.579615
H -0.955288 2.558761 -0.320488
H -2.712921 3.899789 1.826990
H -1.739689 2.440683 2.079333
H -0.939514 3.993562 1.708374

4TS9-10C

Geometry with 89 atoms:
Total energy: -3203.734146480
Cr 0.135632 -1.330740 0.675795
P 1.561345 0.387679 -0.764743
P -1.674813 -0.057010 -0.505339
C -0.935096 1.006563 -1.858353
C 0.474863 0.567695 -2.268636
H -1.603744 1.019955 -2.730931
H -0.910263 2.029392 -1.454666
H 0.446446 -0.402007 -2.786553
H 0.919803 1.301186 -2.959354
C 3.219182 -0.071493 -1.414569
C 3.337176 -0.578365 -2.723121
C 4.368250 -0.006188 -0.581097
C 4.565180 -1.018829 -3.218575
H 2.467210 -0.633950 -3.378541
C 5.591581 -0.450172 -1.107671
C 5.697426 -0.952290 -2.406038
H 4.633206 -1.406735 -4.237649
H 6.488792 -0.400958 -0.487935
H 6.666660 -1.289269 -2.781633
C 1.681004 2.140355 -0.218083
C 2.530750 3.058221 -0.858479
C 0.867416 2.579858 0.838505
C 2.565414 4.390935 -0.440902
H 3.174810 2.729920 -1.678457
C 0.897069 3.915842 1.248699
H 0.194109 1.883660 1.342175
C 1.749556 4.821911 0.612042
H 3.233402 5.097645 -0.939532
H 0.253133 4.244795 2.067998
H 1.780326 5.865084 0.935893
C -2.697899 1.065150 0.532616
C -3.732314 1.902742 0.045885
C -2.403864 1.054666 1.909888
C -4.423619 2.698880 0.976265
C -3.099185 1.857916 2.811975
C -4.118466 2.686750 2.337322
H -5.229337 3.343959 0.614743
H -2.853978 1.826580 3.876112
H -4.682464 3.318700 3.027881
C -2.843338 -1.189010 -1.349931
C -4.042251 -1.571844 -0.724701
C -2.506562 -1.753483 -2.592538
C -4.891794 -2.495706 -1.339038
H -4.323182 -1.138811 0.237818
C -3.361042 -2.674494 -3.203604
H -1.575411 -1.481111 -3.093681
C -4.554812 -3.048204 -2.578301
H -5.824433 -2.781066 -0.846293
H -3.091758 -3.102146 -4.172490
H -5.222280 -3.768333 -3.057588
C 1.957738 -2.119555 1.639881
C 1.454319 -1.073016 2.641724
C 1.058534 -1.611549 4.021235
C -0.027499 -2.691316 4.028103
C -1.327117 -2.281473 3.323205
C -1.293728 -2.383154 1.793992
H 2.201742 -3.042671 2.174309
H 2.843481 -1.766250 1.105504
H 2.233806 -0.302738 2.751696
H 0.592486 -0.416940 2.286153
H 1.972597 -2.000786 4.501328
H 0.724829 -0.760052 4.639619
H -0.237482 -2.945490 5.080174
H 0.356919 -3.619734 3.568430
H -2.142318 -2.926379 3.702517
H -1.602751 -1.259569 3.645996
H -1.142183 -3.441492 1.513169
H -2.284945 -2.113937 1.391758
C 0.291044 -2.793063 -0.799075
C 1.241130 -3.336716 0.114767
H 0.670079 -2.403109 -1.749496
H -0.701070 -3.251281 -0.853407
H 0.908716 -4.151528 0.762281
H 2.280342 -3.428304 -0.211346
H -1.626741 0.388115 2.284989
C -4.128529 2.017672 -1.412296
C -3.681341 3.338644 -2.054729
H -5.226956 1.943223 -1.478107
H -3.743697 1.168540 -1.991425
H -4.123238 4.204109 -1.536076
H -2.587343 3.458335 -2.018076
H -3.993657 3.383980 -3.110173
C 4.310994 0.562226 0.825643
C 5.207799 -0.116546 1.862713
H 3.272306 0.534329 1.184812
H 4.553004 1.639029 0.777187
H 6.277777 0.026436 1.649045
H 5.022697 0.309144 2.861556
H 5.019586 -1.201123 1.914073

catalyst_model_A-01
Geometry with 53 atoms:
Total energy: -2731.334953030
P 1.763143 0.015800 0.231112
P -1.731496 -0.085952 0.238173
C -0.660127 0.335964 -1.234318
C 0.695757 -0.386478 -1.255240
H -1.219404 0.139644 -2.163040
H -0.520383 1.428288 -1.188720
H 0.560431 -1.480500 -1.251397
H 1.242109 -0.120559 -2.174011
C 3.191725 -1.122406 0.097151
C 3.557776 -1.775996 -1.092513
C 3.954636 -1.337444 1.258887
C 4.666363 -2.627872 -1.113583
H 2.989104 -1.625524 -2.012069
C 5.067205 -2.180328 1.231652
H 3.675307 -0.839002 2.192151
C 5.422666 -2.829853 0.044753
H 4.941452 -3.134093 -2.042229
H 5.653705 -2.336687 2.140283
H 6.288368 -3.496334 0.023628
C 2.413292 1.688787 -0.177019
C 3.616422 1.885603 -0.875177
C 1.653021 2.807974 0.207463
C 4.041197 3.179316 -1.190572
H 4.228533 1.030393 -1.170257
C 2.075304 4.099188 -0.118924
H 0.722787 2.673933 0.768153
C 3.271745 4.286249 -0.818081
H 4.980803 3.322812 -1.729927
H 1.473627 4.960807 0.180902
H 3.608128 5.295760 -1.066652
C -2.457008 -1.730485 -0.142254
C -3.208632 -2.348351 0.874596
C -2.293756 -2.394637 -1.369063
C -3.798941 -3.594935 0.662894
H -3.341649 -1.844656 1.837189
C -2.877269 -3.649726 -1.574143
H -1.714125 -1.943101 -2.176247
C -3.631765 -4.249799 -0.562824
H -4.388600 -4.059292 1.457132
H -2.742895 -4.157587 -2.532400
H -4.088650 -5.228654 -0.727505
C -3.117028 1.105375 0.064596
C -4.134231 0.926843 -0.888048
C -3.131611 2.244228 0.886276
C -5.144145 1.882650 -1.019980
H -4.141872 0.036525 -1.521853
C -4.140633 3.201586 0.747876
H -2.354476 2.381514 1.644733
C -5.147111 3.020896 -0.205587
H -5.934428 1.737846 -1.760780
H -4.145764 4.085123 1.390993
H -5.940429 3.765202 -0.310290
Cr 0.016021 -0.089902 2.105001

catalyst_model_A-02
Geometry with 53 atoms:
Total energy: -2731.335106320
P -1.741603 -0.100682 0.247210
P 1.741603 0.100682 0.247208
C 0.682290 -0.353068 -1.228982
C -0.682291 0.353068 -1.228981
H 1.227561 -0.102185 -2.152352
H 0.553015 -1.447907 -1.207900
H -0.553016 1.447907 -1.207899
H -1.227562 0.102185 -2.152351
C -3.202784 0.997027 0.135849
C -3.532008 1.744175 -1.008077

C	-4.033341	1.076195	1.268633
C	-4.672947	2.553296	-1.014143
H	-2.910188	1.700874	-1.904163
C	-5.177627	1.875234	1.254452
H	-3.783018	0.504886	2.167949
C	-5.497759	2.617711	0.112382
H	-4.920192	3.131862	-1.907689
H	-5.818538	1.923239	2.138242
H	-6.389908	3.248618	0.102262
C	-2.352439	-1.777410	-0.203400
C	-3.533273	-1.979328	-0.937376
C	-1.581905	-2.890660	0.176398
C	-3.926766	-3.272987	-1.290850
H	-4.151320	-1.127754	-1.231351
C	-1.972891	-4.181890	-0.187662
H	-0.668287	-2.752479	0.763058
C	-3.147496	-4.374315	-0.921397
H	-4.849098	-3.421270	-1.857989
H	-1.363958	-5.039203	0.109907
H	-3.459269	-5.383960	-1.199846
C	3.202785	-0.997027	0.135847
C	4.033342	-1.076193	1.268631
C	3.532009	-1.744175	-1.008078
C	5.177628	-1.875232	1.254451
H	3.783019	-0.504884	2.167947
C	4.672948	-2.553296	-1.014144
H	2.910189	-1.700874	-1.904164
C	5.497761	-2.617710	0.112382
H	5.818539	-1.923236	2.138241
H	4.920193	-3.131862	-1.907690
H	6.389909	-3.248616	0.102261
C	2.352437	1.777410	-0.203400
C	3.533272	1.979329	-0.937377
C	1.581903	2.890660	0.176399
C	3.926764	3.272989	-1.290850
H	4.151319	1.127756	-1.231353
C	1.972889	4.181890	-0.187660
H	0.668286	2.752478	0.763059
C	3.147493	4.374316	-0.921396
H	4.849095	3.421273	-1.857989
H	1.363955	5.039202	0.109910
H	3.459266	5.383961	-1.199844
Cr	0.000002	-0.000003	2.128065

catalyst_model_A-03
Geometry with 53 atoms:
Total energy: -2731.335323690

P	1.744777	0.039447	0.214292
P	-1.744799	-0.039517	0.214302
C	-0.662130	-0.389881	-1.268599
C	0.662092	0.389742	-1.268617
H	-0.481092	-1.476686	-1.237551
H	-1.230141	-0.200074	-2.193324
H	1.230098	0.199902	-2.193338
H	0.481048	1.476548	-1.237612
C	2.478208	-1.616020	-0.088832
C	2.431297	-2.280779	-1.325468
C	3.122071	-2.238349	0.996905
C	3.018016	-3.542366	-1.470068
H	1.943853	-1.823506	-2.188424
C	3.717995	-3.491539	0.846373
H	3.164218	-1.732363	1.966741
C	3.663322	-4.147900	-0.388294
H	2.973198	-4.051523	-2.435914
H	4.222977	-3.959662	1.694887
H	4.123024	-5.132188	-0.506108
C	3.115946	1.239241	-0.007996
C	4.296558	0.922132	-0.699283
C	2.954162	2.528598	0.528387
C	5.295437	1.887294	-0.856241
H	4.440450	-0.078655	-1.113177
C	3.950871	3.492586	0.360819
H	2.044408	2.782445	1.081998
C	5.124225	3.171693	-0.330147
H	6.212795	1.633144	-1.393155
H	3.815836	4.493568	0.778061
H	5.908533	3.922542	-0.453835
C	-2.478119	1.616001	-0.088822
C	-3.121965	2.238359	0.996908
C	-2.431132	2.280773	-1.325447
C	-3.717804	3.491590	0.846377
H	-3.164167	1.732364	1.966737
C	-3.017766	3.542400	-1.470046
H	-1.943692	1.823482	-2.188397
C	-3.663060	4.147962	-0.388280
H	-4.222775	3.959735	1.694885
H	-2.972890	4.051567	-2.435884
H	-4.122694	5.132281	-0.506094
C	-3.116043	-1.239225	-0.007987
C	-2.954339	-2.528592	0.528396
C	-4.296636	-0.922041	-0.699271
C	-3.951109	-3.492518	0.360830
H	-2.044599	-2.782497	1.082005
C	-5.295577	-1.887140	-0.856226
H	-4.440467	0.078755	-1.113162
C	-5.124445	-3.171550	-0.330133
H	-3.816137	-4.493507	0.778072
H	-6.212920	-1.632932	-1.393137
H	-5.908801	-3.922349	-0.453818
Cr	-0.000008	-0.000091	2.083300

catalyst_model_A-04
Geometry with 53 atoms:
Total energy: -2731.334835830

P	1.737470	-0.156069	0.249703
P	-1.754422	-0.054773	0.244822
C	-0.687438	-0.528133	-1.216118
C	0.646551	0.232096	-1.227076
H	-0.522771	-1.617373	-1.161876
H	-1.238880	-0.322122	-2.147279
H	1.203907	0.015711	-2.151413
H	0.468721	1.319301	-1.217211
C	2.548640	-1.737938	-0.205184
C	3.140250	-1.939895	-1.466042
C	2.571327	-2.781564	0.734716
C	3.737882	-3.162848	-1.775641
H	3.147768	-1.137334	-2.207883
C	3.170483	-4.006055	0.423234
H	2.121780	-2.636157	1.721806
C	3.752657	-4.197425	-0.832487
H	4.196572	-3.309365	-2.756656
H	3.182861	-4.810298	1.162854
H	4.221546	-5.153438	-1.078240
C	3.031772	1.144900	0.146597
C	4.403036	0.845715	0.100824
C	2.627029	2.492802	0.199910
C	5.348357	1.876791	0.088517
H	4.740688	-0.192068	0.069842
C	3.574200	3.517809	0.180116
H	1.564984	2.751799	0.252802
C	4.938746	3.212115	0.123686
H	6.412467	1.631061	0.047660
H	3.245829	4.559708	0.210863
H	5.680306	4.014534	0.109609
C	-3.240815	-1.118513	0.117781
C	-4.107815	-1.139162	1.225680
C	-3.549095	-1.901045	-1.007863
C	-5.267627	-1.914915	1.203500
H	-3.873173	-0.541244	2.111897
C	-4.707265	-2.685530	-1.021909
H	-2.895692	-1.907160	-1.882375
C	-5.568095	-2.691794	0.078929
H	-5.936569	-1.918327	2.067667
H	-4.938296	-3.292100	-1.901094
H	-6.472698	-3.304554	0.063192
C	-2.326043	1.632159	-0.221554
C	-3.300883	1.832415	-1.213652
C	-1.740263	2.747646	0.399931
C	-3.673814	3.127635	-1.580020
H	-3.777517	0.975057	-1.696049
C	-2.110311	4.043587	0.027159
H	-0.994729	2.606437	1.189274
C	-3.077766	4.233898	-0.963522
H	-4.436358	3.274607	-2.348959
H	-1.648809	4.904196	0.517621
H	-3.373583	5.245688	-1.251444
Cr	-0.026094	-0.200102	2.122519

catalyst_model_B-01
Geometry with 61 atoms:
Total energy: -2960.241203040

P	1.713964	-0.154305	0.085174
P	-1.713981	0.154217	0.085290
C	-0.706610	-0.299663	-1.425710
C	0.706466	0.299464	-1.425761
H	-0.659237	-1.399052	-1.441324
H	-1.244528	0.029381	-2.328521
H	1.244320	-0.029676	-2.328569
H	0.659167	1.398859	-1.441448
C	2.243595	-1.881467	-0.275762
C	3.475493	-2.194531	-0.866651
C	1.366101	-2.937267	0.070814
C	3.835730	-3.520729	-1.123395
H	4.163967	-1.388353	-1.130147
C	1.721489	-4.266388	-0.190424
C	2.955227	-4.549568	-0.786287
H	4.798891	-3.745505	-1.586470
H	1.049665	-5.084367	0.068776
H	3.224179	-5.590143	-0.983995
C	3.238742	0.851832	-0.063762
C	3.626625	1.527230	-1.233523
C	4.039374	0.967320	1.087707
C	4.790553	2.303353	-1.245891
H	3.030838	1.454314	-2.145135
C	5.207779	1.731007	1.068529
H	3.741899	0.454174	2.007492
C	5.583070	2.405042	-0.099078
H	5.081008	2.827046	-2.160151
H	5.823244	1.806685	1.968381
H	6.492716	3.010379	-0.113588
C	-2.243491	1.881392	-0.275807
C	-3.475264	2.194420	-0.866991
C	-1.366031	2.937206	0.070819
C	-3.835404	3.520589	-1.123994
H	-4.163713	1.388233	-1.130516
C	-1.721328	4.266307	-0.190704
C	-2.954927	4.549444	-0.786863
H	-4.798467	3.745330	-1.587291
H	-1.049506	5.084296	0.068471
H	-3.223789	5.590000	-0.984796
C	-3.238929	-0.851684	-0.063556
C	-3.626157	-1.528127	-1.232932
C	-4.040336	-0.965971	1.087498
C	-4.790207	-2.304073	-1.245352
H	-3.029762	-1.456182	-2.144216
C	-5.208851	-1.729482	1.068247
H	-3.743415	-0.451985	2.006994
C	-5.583502	-2.404545	-0.098979
H	-5.080149	-2.828543	-2.159331
H	-5.824946	-1.804195	1.967749
H	-6.493257	-3.009717	-0.113516
O	0.185058	-2.576803	0.657834
O	-0.185126	2.576803	0.658097
C	-0.814711	-3.557713	0.904898
H	-1.677419	-3.020859	1.320524
H	-1.123756	-4.059653	-0.027404
H	-0.472045	-4.313284	1.632104
C	0.814528	3.557734	0.905448
H	0.471568	4.313425	1.632392
H	1.677040	3.020947	1.321561
H	1.124007	4.059526	-0.026794
Cr	0.000338	-0.000273	1.954130

catalyst_model_B-02
Geometry with 61 atoms:
Total energy: -2960.236402670

P	2.015178	0.236903	0.179291
P	-1.388777	0.544138	-0.125320
C	-0.217914	0.360625	-1.577606
C	1.163486	0.977324	-1.314569
H	-0.118419	-0.719925	-1.770520
H	-0.663464	0.816942	-2.475312
H	1.802027	0.832337	-2.200526
H	1.082483	2.062716	-1.135265
C	2.304596	-1.502603	-0.373396
C	3.406480	-1.850992	-1.169068
C	1.386477	-2.515673	-0.009406
C	3.600783	-3.163536	-1.604635
H	4.126647	-1.078867	-1.449883
C	1.574945	-3.832681	-0.447728
C	2.680866	-4.148725	-1.242472
H	4.465472	-3.412830	-2.223299
H	0.871956	-4.618778	-0.174780

H	2.818502	-5.179996	-1.576390
C	3.687633	0.986388	0.189465
C	4.142061	1.903906	-0.772299
C	4.541990	0.626753	1.248790
C	5.429150	2.444876	-0.675797
H	3.506095	2.204669	-1.606652
C	5.828976	1.157921	1.333867
H	4.196923	-0.080058	2.009578
C	6.274982	2.071511	0.371369
H	5.772081	3.158506	-1.429102
H	6.485098	0.863634	2.156780
H	7.280826	2.492837	0.440662
C	-2.756848	-0.608704	-0.523376
C	-2.995127	-1.116949	-1.808862
C	-3.596429	-1.026792	0.539067
C	-4.037286	-2.017343	-2.050947
H	-2.366072	-0.803895	-2.643866
C	-4.645435	-1.924849	0.297940
C	-4.859069	-2.413503	-0.994809
H	-4.207859	-2.398487	-3.059922
H	-5.297614	-2.249653	1.108336
H	-5.681017	-3.111860	-1.170921
C	-2.078464	2.232716	-0.358125
C	-3.225784	2.493494	-1.125497
C	-1.399180	3.305793	0.245662
C	-3.678059	3.805887	-1.288854
H	-3.771730	1.671365	-1.594266
C	-1.846793	4.617904	0.070444
H	-0.516814	3.113978	0.864527
C	-2.989184	4.869270	-0.695977
H	-4.574765	3.999047	-1.883163
H	-1.308480	5.444042	0.541785
H	-3.346605	5.893743	-0.826086
O	0.321054	-2.145363	0.777599
O	-3.301671	-0.527000	1.767302
C	-0.722510	-3.084879	1.040647
H	-1.481743	-2.541362	1.617107
H	-1.177158	-3.446919	0.104891
H	-0.353750	-3.937684	1.633967
C	-4.150970	-0.807784	2.869554
H	-4.164049	-1.884788	3.112535
H	-3.739399	-0.254231	3.724615
H	-5.182591	-0.463457	2.684216
Cr	0.127171	0.094007	1.875495

catalyst_model_B-03
Geometry with 61 atoms:
Total energy: -2960.235541180

P	-1.955924	0.364858	-0.198369
P	1.482850	0.071119	-0.396759
C	0.491832	0.042675	1.195176
C	-0.765737	0.919442	1.132855
H	0.217204	-1.005470	1.391754
H	1.149756	0.364956	2.013977
H	-1.279997	0.906423	2.107373
H	-0.496548	1.965387	0.910521
C	-2.526571	-1.267966	0.447989
C	-3.490516	-1.352942	1.464689
C	-1.988692	-2.466707	-0.075544
C	-3.919912	-2.586295	1.957742
H	-3.919169	-0.432742	1.869181
C	-2.420682	-3.707269	0.412771
C	-3.381833	-3.759480	1.426351
H	-4.671814	-2.628978	2.748552
H	-2.018990	-4.637047	0.012412
H	-3.709920	-4.733297	1.797824
C	-3.423599	1.446631	-0.011638
C	-4.555467	1.144841	-0.793057
C	-3.452539	2.576452	0.822084
C	-5.696034	1.944645	-0.727613
H	-4.547544	0.270879	-1.451322
C	-4.595153	3.383201	0.875488
H	-2.592343	2.841076	1.439335
C	-5.717871	3.069010	0.106590
H	-6.570900	1.692555	-1.332167
H	-4.605893	4.259359	1.528681
H	-6.609546	3.698812	0.154174
C	2.346909	1.686290	-0.360023
C	2.143029	2.579512	-1.422698
C	3.198657	2.077700	0.706077
C	2.753890	3.835517	-1.449994
H	1.492480	2.277888	-2.249698
C	3.818604	3.336495	0.677239
C	3.590374	4.204322	-0.395024
H	2.581028	4.515145	-2.286873
H	4.476330	3.648829	1.487978
H	4.078952	5.181977	-0.399637
C	2.768103	-1.217030	-0.147557
C	2.398739	-2.492774	0.314676
C	4.105410	-0.987630	-0.512207
C	3.350951	-3.509733	0.426706
H	1.365033	-2.702223	0.599153
C	5.053351	-2.007908	-0.402630
H	4.413682	-0.004710	-0.876157
C	4.681200	-3.271102	0.068410
H	3.050919	-4.492842	0.798840
H	6.091469	-1.812153	-0.683230
H	5.425496	-4.066278	0.156682
O	-1.034739	-2.355813	-1.061614
O	3.361529	1.182044	1.703494
C	-0.477003	-3.540779	-1.632689
H	0.283084	-3.208290	-2.352053
H	0.014115	-4.165781	-0.870515
H	-1.246777	-4.130251	-2.157609
C	4.287083	1.434642	2.749086
H	3.999201	2.318393	3.344485
H	4.269328	0.546472	3.394347
H	5.309412	1.573248	2.357496
Cr	-0.371891	-0.178058	-2.115881

catalyst_model_B-04
Geometry with 61 atoms:
Total energy: -2960.236792510

P	1.650736	0.157654	-0.177891
P	-1.650534	-0.157380	-0.178259
C	-0.655388	-0.396291	-1.748445
C	0.655775	0.396720	-1.748252
H	-0.447627	-1.475561	-1.822180
H	-1.268367	-0.123459	-2.622099
H	1.268954	0.123980	-2.621787
H	0.448050	1.476001	-1.821936
C	2.106317	-1.625916	-0.280284
C	2.766036	-2.139963	-1.409044
C	1.758695	-2.519905	0.759999
C	3.082974	-3.493980	-1.518253
H	3.047224	-1.456294	-2.214014
C	2.072134	-3.881994	0.654152
C	2.732291	-4.359833	-0.480625
H	3.600350	-3.868594	-2.403895
H	1.807449	-4.581208	1.445513
H	2.970773	-5.424096	-0.547143
C	3.195148	1.090317	-0.515872
C	4.472335	0.540337	-0.310960
C	3.089007	2.444303	-0.889685
C	5.616470	1.321907	-0.498949
H	4.580458	-0.503494	-0.009047
C	4.235088	3.218141	-1.082525
H	2.107193	2.905684	-1.030132
C	5.502986	2.658984	-0.889622
H	6.603222	0.878721	-0.342173
H	4.137002	4.264418	-1.383109
H	6.399274	3.265468	-1.040638
C	-2.106457	1.626080	-0.280549
C	-2.766187	2.140066	-1.409327
C	-1.759179	2.520056	0.759870
C	-3.083568	3.493991	-1.518400
H	-3.047013	1.456420	-2.214442
C	-2.073115	3.882042	0.654184
C	-2.733334	4.359805	-0.480594
H	-3.600933	3.868548	-2.404072
H	-1.808802	4.581262	1.445661
H	-2.972210	5.423990	-0.546965
C	-3.194747	-1.090421	-0.516098
C	-3.088298	-2.444438	-0.889710
C	-4.472059	-0.540723	-0.311239
C	-4.234200	-3.218585	-1.082380
H	-2.106401	-2.905631	-1.030177
C	-5.616016	-1.322598	-0.499070
H	-4.580441	0.503128	-0.009492
C	-5.502232	-2.659712	-0.889522
H	-4.135859	-4.264888	-1.382791
H	-6.602864	-0.879607	-0.342344
H	-6.398376	-3.266444	-1.040388
O	1.097663	-2.013247	1.863544
O	-1.098051	2.013461	1.863396
C	0.840159	-2.877490	2.978409
H	0.390816	-2.250183	3.759259
H	0.132465	-3.677108	2.706133
H	1.775618	-3.313905	3.362704
C	-0.840204	2.877842	2.978081
H	-1.775590	3.314000	3.362852
H	-0.390212	2.250716	3.758698
H	-0.132897	3.677660	2.705387
Cr	-0.000157	0.000091	1.774900

catalyst_model_B-05
Geometry with 61 atoms:
Total energy: -2960.234203470

P	-1.450276	0.529768	-0.390738
P	2.007297	0.143767	-0.219232
C	0.909479	0.746807	1.169198
C	-0.491514	0.116894	1.163549
H	1.402532	0.537111	2.131958
H	0.836436	1.842667	1.063933
H	-0.436980	-0.980745	1.224087
H	-1.056911	0.462122	2.038186
C	-2.942493	-0.544397	-0.425012
C	-3.396521	-0.916345	-1.701309
C	-3.650703	-1.021694	0.705943
C	-4.507283	-1.743690	-1.878410
H	-2.857594	-0.544437	-2.578100
C	-4.755798	-1.870678	0.531939
C	-5.177006	-2.224969	-0.752310
H	-4.840878	-2.011698	-2.882993
H	-5.300193	-2.250912	1.395758
H	-6.042688	-2.882210	-0.866137
C	-2.034542	2.244941	-0.071029
C	-2.931653	2.553095	0.968602
C	-1.544169	3.281822	-0.881593
C	-3.323602	3.874993	1.187582
H	-3.320610	1.756642	1.605680
C	-1.933636	4.606020	-0.655555
H	-0.852667	3.054243	-1.698782
C	-2.824762	4.903174	0.378601
H	-4.023099	4.105870	1.995058
H	-1.543645	5.404543	-1.291619
H	-3.134063	5.936506	0.554426
C	2.387661	-1.583503	0.302720
C	3.503021	-1.896627	1.092983
C	1.524287	-2.629580	-0.099922
C	3.765012	-3.211543	1.485888
H	4.179254	-1.097172	1.404194
C	1.781000	-3.948332	0.297477
C	2.900186	-4.231258	1.086866
H	4.639295	-3.434835	2.100996
H	1.120445	-4.760854	-0.002705
H	3.091267	-5.264273	1.387580
C	3.589324	1.042179	-0.002947
C	4.575567	0.845269	-0.987627
C	3.857047	1.914292	1.065195
C	5.808218	1.492418	-0.897650
H	4.377899	0.173915	-1.828688
C	5.089693	2.571722	1.145182
H	3.115800	2.088656	1.846991
C	6.066814	2.360922	0.169225
H	6.567658	1.324451	-1.665315
H	5.286366	3.249145	1.979893
H	7.029108	2.874129	0.237276
O	-3.213337	-0.616812	1.922220
O	0.448637	-2.281552	-0.876416
C	-3.848024	-1.082342	3.103548
H	-3.306403	-0.624541	3.942051
H	-4.906179	-0.772197	3.147196
H	-3.784788	-2.180657	3.192656
C	-0.530504	-3.267277	-1.194015
H	-0.988556	-3.682925	-0.281101
H	-1.308268	-2.758238	-1.775798
H	-0.100668	-4.084007	-1.797495
Cr	0.363743	0.137904	-2.151616

catalyst_model_B-06
Geometry with 61 atoms:
Total energy: -2960.233647190

P	1.896347	0.581374	0.084400
P	-1.555322	0.428762	-0.111684
C	-0.474077	1.332601	-1.343089
C	0.892930	0.648580	-1.506695
H	-0.988862	1.385928	-2.315944
H	-0.354973	2.362663	-0.968040
H	0.760251	-0.396711	-1.826529
H	1.483084	1.144520	-2.292890
C	2.794865	-1.017634	-0.066858
C	3.797179	-1.201951	-1.032862
C	2.453097	-2.105026	0.770719
C	4.451735	-2.425472	-1.177674
H	4.072138	-0.363323	-1.677376
C	3.109313	-3.335611	0.629184
C	4.101880	-3.488162	-0.342822
H	5.227922	-2.547091	-1.936137
H	2.859337	-4.183057	1.265709
H	4.603715	-4.453714	-0.441874
C	3.194089	1.863918	-0.112957
C	4.425252	1.722396	0.553871
C	2.936838	3.049841	-0.823183
C	5.383022	2.736394	0.492507
H	4.645308	0.809615	1.113627
C	3.897443	4.064513	-0.876922
H	1.985808	3.194308	-1.342199
C	5.122820	3.910560	-0.222627
H	6.339703	2.607158	1.005013
H	3.685629	4.978763	-1.437094
H	5.873681	4.703031	-0.268882
C	-3.099314	1.407163	-0.045806
C	-3.297535	2.628356	-0.704579
C	-4.134971	0.897131	0.776471
C	-4.495492	3.336566	-0.559281
H	-2.518181	3.040933	-1.347336
C	-5.338646	1.599619	0.915222
C	-5.508716	2.817717	0.247843
H	-4.634668	4.285873	-1.080807
H	-6.142046	1.209859	1.540335
H	-6.449442	3.361541	0.364079
C	-1.999861	-1.102878	-1.033033
C	-3.014739	-1.116067	-2.003656
C	-1.271066	-2.277684	-0.784260
C	-3.292095	-2.286868	-2.713788
H	-3.595060	-0.211032	-2.201505
C	-1.544311	-3.445271	-1.503083
H	-0.485459	-2.282100	-0.023298
C	-2.556731	-3.451745	-2.467229
H	-4.086518	-2.289812	-3.464510
H	-0.967951	-4.352681	-1.305542
H	-2.776036	-4.365314	-3.025503
O	1.455810	-1.910127	1.705802
O	-3.863190	-0.282919	1.383608
C	1.100828	-2.987293	2.576782
H	0.301229	-2.609760	3.228373
H	0.719217	-3.851979	2.009866
H	1.956371	-3.295888	3.199175
C	-4.871563	-0.950303	2.123633
H	-4.430605	-1.898077	2.460961
H	-5.186021	-0.366280	3.006307
H	-5.754266	-1.169402	1.498378
Cr	0.059473	0.125167	1.806777

catalyst_model_B-07
Geometry with 61 atoms:
Total energy: -2960.233829510

P	1.424413	-0.233510	-0.327807
P	-1.996402	-0.414111	-0.143858
C	-0.857527	-1.029281	1.208877
C	0.458101	-0.241395	1.270733
H	-1.379691	-0.973213	2.177908
H	-0.660488	-2.092622	0.998272
H	0.260173	0.822408	1.481918
H	1.099088	-0.607436	2.085432
C	2.723926	1.025091	-0.045346
C	2.777673	2.139903	-0.892906
C	3.677984	0.905163	0.995686
C	3.752050	3.128718	-0.731875
H	2.041341	2.224899	-1.697359
C	4.664352	1.890913	1.152284
C	4.692516	2.992696	0.291463
H	3.781457	3.990545	-1.401889
H	5.408353	1.810101	1.944953
H	5.465629	3.753084	0.428767
C	2.299621	-1.850607	-0.411054
C	2.257957	-2.821348	0.601660
C	3.014265	-2.124857	-1.590417
C	2.918986	-4.042282	0.434816
H	1.721232	-2.632002	1.532771
C	3.688293	-3.337603	-1.747945
H	3.050975	-1.379110	-2.390888
C	3.637698	-4.302186	-0.735931
H	2.877334	-4.792485	1.228713
H	4.248939	-3.533320	-2.665503
H	4.156109	-5.255986	-0.861142
C	-2.383886	1.296077	0.429382
C	-3.099022	1.501463	1.620439
C	-1.941129	2.425157	-0.298691
C	-3.372174	2.784522	2.094268
H	-3.454533	0.632481	2.180655
C	-2.212199	3.716958	0.175623
C	-2.923436	3.888096	1.365851
H	-3.930381	2.921324	3.022745
H	-1.876847	4.597930	-0.369693
H	-3.126131	4.901210	1.721532
C	-3.563202	-1.332228	0.111592
C	-3.598478	-2.603365	0.710206
C	-4.755604	-0.786098	-0.400470
C	-4.804070	-3.307545	0.800072
H	-2.691824	-3.059334	1.112686
C	-5.956071	-1.490610	-0.303478
H	-4.748266	0.202219	-0.868626
C	-5.984030	-2.755073	0.296207
H	-4.817872	-4.293808	1.270721
H	-6.875156	-1.049952	-0.697909
H	-6.924249	-3.306883	0.369716
O	3.561554	-0.180235	1.791266
O	-1.243294	2.205572	-1.467177
C	4.552883	-0.461403	2.765995
H	4.276330	-1.424183	3.216249
H	5.553431	-0.554420	2.309820
H	4.579369	0.310140	3.554993
C	-0.783013	3.327029	-2.224048
H	-0.065657	3.933247	-1.647834
H	-0.277879	2.918046	-3.109708
H	-1.623415	3.957825	-2.556110
Cr	-0.388684	0.011477	-2.064454

catalyst_model_B-08
Geometry with 61 atoms:
Total energy: -2960.234021120

P	-1.548310	0.098675	-0.424741
P	1.936569	0.295354	-0.174205
C	0.761712	-0.189925	1.201087
C	-0.583759	0.543079	1.121627
H	0.628593	-1.278760	1.106817
H	1.241240	-0.011134	2.175669
H	-1.210709	0.316067	1.995010
H	-0.434185	1.634420	1.108753
C	-2.415854	-1.456821	-0.001563
C	-2.211804	-2.579755	-0.817219
C	-3.274918	-1.577276	1.121633
C	-2.830271	-3.802973	-0.547034
H	-1.558879	-2.485694	-1.689854
C	-3.902233	-2.803629	1.391875
C	-3.673685	-3.904433	0.561065
H	-2.660230	-4.663611	-1.197169
H	-4.567077	-2.907373	2.249013
H	-4.169249	-4.851995	0.787288
C	-2.819458	1.414048	-0.572493
C	-4.184970	1.127078	-0.727889
C	-2.390134	2.752026	-0.642273
C	-5.103733	2.160996	-0.928647
H	-4.538075	0.094373	-0.692000
C	-3.312615	3.782848	-0.835917
H	-1.328347	3.000095	-0.547069
C	-4.672961	3.490190	-0.978567
H	-6.164624	1.924655	-1.044399
H	-2.966033	4.818482	-0.879176
H	-5.394585	4.296231	-1.132122
C	3.348207	-0.847989	0.069372
C	4.617634	-0.449944	0.507689
C	3.133520	-2.206491	-0.267444
C	5.655752	-1.379051	0.633543
H	4.799434	0.597261	0.757548
C	4.168514	-3.139605	-0.134786
C	5.424608	-2.718129	0.316846
H	6.638781	-1.054248	0.981185
H	4.010257	-4.189362	-0.381517
H	6.227902	-3.452301	0.416788
C	2.529094	1.964664	0.304643
C	2.665714	2.931020	-0.706858
C	2.827797	2.321257	1.632557
C	3.091899	4.226946	-0.401448
H	2.439000	2.665873	-1.743969
C	3.250144	3.617444	1.936778
H	2.740329	1.587615	2.437359
C	3.382055	4.571576	0.921583
H	3.195296	4.968253	-1.197648
H	3.478859	3.883880	2.971691
H	3.711528	5.585062	1.163544
O	-3.440761	-0.467020	1.871305
O	1.881397	-2.513127	-0.712724
C	-4.385025	-0.451693	2.931152
H	-5.401652	-0.679753	2.567583
H	-4.112988	-1.162480	3.730595
H	-4.371411	0.568061	3.337866
C	1.530566	-3.867499	-0.954937
H	1.663391	-4.486081	-0.050993
H	0.466794	-3.867252	-1.227107
H	2.118670	-4.299172	-1.783147
Cr	0.350592	0.008828	-2.137969

catalyst_model_B-09
Geometry with 61 atoms:
Total energy: -2960.234512260

P	-1.381288	0.788500	0.125108
P	1.985454	0.460659	-0.198659
C	1.192899	1.463815	1.178331
C	-0.190596	0.923114	1.573111
H	1.862933	1.460035	2.053183
H	1.123178	2.505347	0.825220
H	-0.083956	-0.090220	1.989334
H	-0.634961	1.555863	2.356658
C	-2.388664	-0.701829	0.491579
C	-2.720226	-1.086051	1.799303
C	-2.852676	-1.490581	-0.587827
C	-3.485099	-2.227930	2.047688
H	-2.384903	-0.475166	2.640971
C	-3.626826	-2.634025	-0.342504
C	-3.935401	-2.996072	0.972246
H	-3.733641	-2.509346	3.073070
H	-3.993161	-3.246218	-1.166411
H	-4.539402	-3.889118	1.150803
C	-2.536325	2.198468	0.354200
C	-3.929811	2.037478	0.282836
C	-2.004630	3.491060	0.521175
C	-4.773402	3.147532	0.388712
H	-4.362320	1.042463	0.155890
C	-2.851857	4.595210	0.634948
H	-0.921783	3.641790	0.564970
C	-4.239340	4.426805	0.567184
H	-5.856277	3.008056	0.338043
H	-2.426600	5.592452	0.773731
H	-4.901884	5.291442	0.653146
C	2.086266	-1.197927	0.598101
C	2.848239	-1.387696	1.762772
C	1.336651	-2.285969	0.093541
C	2.874636	-2.615643	2.423832
H	3.439852	-0.554852	2.151468
C	1.354818	-3.520339	0.760611
C	2.120506	-3.677062	1.917981
H	3.476202	-2.741891	3.326354
H	0.771499	-4.362506	0.391224
H	2.123114	-4.644265	2.426437
C	3.716719	1.069308	-0.243500
C	4.777629	0.184814	-0.510734
C	3.991596	2.444068	-0.123551
C	6.083414	0.664026	-0.637967
H	4.586961	-0.886518	-0.609947
C	5.300182	2.917969	-0.250961
H	3.188846	3.159530	0.069818
C	6.349774	2.030759	-0.506885
H	6.898142	-0.036577	-0.837754

H 5.499160 3.987682 -0.147575
H 7.372329 2.403309 -0.604283
O -2.502055 -1.087726 -1.845137
O 0.600420 -2.080323 -1.045733
C -3.148500 -1.661384 -2.973161
H -2.793323 -1.102168 -3.849684
H -2.892337 -2.726996 -3.101405
H -4.244265 -1.557917 -2.902039
C -0.052274 -3.188181 -1.661958
H -0.865075 -3.577874 -1.028656
H -0.476668 -2.811578 -2.600789
H 0.663700 -3.994046 -1.891965
Cr 0.102876 0.275995 -1.881008

catalyst_model_B-10
Geometry with 61 atoms:
Total energy: -2960.234366340
P -1.437509 0.539218 0.125354
P 1.975791 0.184522 -0.151701
C 1.095851 0.886593 1.345696
C -0.294188 0.269970 1.575392
H 1.721833 0.725880 2.237482
H 1.017503 1.974918 1.183562
H -0.222458 -0.821634 1.702480
H -0.725198 0.666584 2.506918
C -2.884642 -0.532024 0.502036
C -3.401537 -0.655842 1.800124
C -3.513817 -1.238599 -0.551672
C -4.512280 -1.458980 2.067095
H -2.933793 -0.108443 2.621402
C -4.633408 -2.041549 -0.286845
C -5.124929 -2.145782 1.017182
H -4.899379 -1.540638 3.084896
H -5.128459 -2.587406 -1.089662
H -5.999479 -2.772730 1.207943
C -2.068802 2.258502 0.320147
C -2.269000 2.881700 1.563683
C -2.378299 2.966534 -0.853688
C -2.767262 4.185595 1.627522
H -2.039212 2.357753 2.494236
C -2.885061 4.267046 -0.788634
H -2.225080 2.491440 -1.827519
C -3.077429 4.879639 0.453198
H -2.915752 4.661658 2.600047
H -3.125105 4.804931 -1.709225
H -3.467137 5.899153 0.506977
C 2.461725 -1.496803 0.432449
C 3.683377 -1.746262 1.074134
C 1.570644 -2.575723 0.224340
C 4.019509 -3.029109 1.514536
H 4.384914 -0.923358 1.228676
C 1.900902 -3.861685 0.670839
C 3.123651 -4.080025 1.313627
H 4.975577 -3.203311 2.012753
H 1.217206 -4.696821 0.522622
H 3.371899 -5.087654 1.655943
C 3.555916 1.108095 -0.237763
C 4.313458 0.964417 -1.414541
C 4.040640 1.936334 0.788675
C 5.537360 1.619850 -1.556374
H 3.941257 0.331240 -2.225721
C 5.261358 2.602691 0.637782
H 3.478947 2.068797 1.715145
C 6.012571 2.443577 -0.529815
H 6.118522 1.494018 -2.473228
H 5.627851 3.246421 1.441318
H 6.966892 2.963868 -0.642414
O -2.968098 -1.113630 -1.795549
O 0.397247 -2.287794 -0.422134
C -3.615114 -1.705548 -2.911835
H -3.021631 -1.427890 -3.793990
H -3.645417 -2.806282 -2.833822
H -4.641618 -1.321006 -3.036316
C -0.584587 -3.306376 -0.590564
H -0.955315 -3.668853 0.382406
H -1.409042 -2.838074 -1.139764
H -0.191508 -4.153986 -1.176599
Cr 0.075671 0.010388 -1.844175

catalyst_model_B-11
Geometry with 61 atoms:
Total energy: -2960.234500250
P -1.393959 0.794877 0.123701
P 1.980031 0.503898 -0.214292
C 1.177834 1.526101 1.140264
C -0.194231 0.970788 1.556790
H 1.849505 1.557731 2.013462
H 1.089969 2.554814 0.753929
H -0.067413 -0.036182 1.982715
H -0.638716 1.602626 2.341186
C -2.372371 -0.709463 0.518959
C -2.684206 -1.081588 1.834841
C -2.828925 -1.523303 -0.544589
C -3.419230 -2.237626 2.106647
H -2.355872 -0.451400 2.664988
C -3.571575 -2.682255 -0.275900
C -3.859050 -3.032766 1.046746
H -3.652418 -2.509456 3.138204
H -3.930669 -3.315117 -1.087252
H -4.439056 -3.937795 1.243707
C -2.587723 2.175408 0.329626
C -2.127231 3.458898 0.674556
C -3.952690 1.992865 0.047825
C -3.017732 4.533084 0.749637
H -1.069446 3.629473 0.893363
C -4.838195 3.071248 0.120689
H -4.332245 1.003262 -0.217680
C -4.375212 4.343098 0.472015
H -2.647984 5.523457 1.027212
H -5.898609 2.913782 -0.092561
H -5.070717 5.183802 0.530835
C 2.102046 -1.143349 0.604187
C 2.882522 -1.308250 1.759868
C 1.363366 -2.247566 0.119675
C 2.930970 -2.526837 2.436897
H 3.470134 -0.463033 2.127932
C 1.403646 -3.472505 0.802850
C 2.183032 -3.603521 1.954523
H 3.545407 -2.634414 3.333161
H 0.827830 -4.327397 0.450910
H 2.202807 -4.563419 2.476296
C 3.712804 1.103688 -0.266588
C 4.055505 2.420866 0.084459
C 4.713081 0.248640 -0.766292
C 5.373658 2.868272 -0.053845
H 3.302756 3.111255 0.470740
C 6.027587 0.698552 -0.897474
H 4.465953 -0.779998 -1.042953
C 6.362183 2.010520 -0.542629
H 5.627011 3.893673 0.227045
H 6.795744 0.020587 -1.278064
H 7.391552 2.361949 -0.646593
O -2.506166 -1.124538 -1.810851
O 0.618707 -2.067334 -1.019272
C -3.112958 -1.763920 -2.925258
H -2.783287 -1.210341 -3.815287
H -2.796680 -2.816907 -3.020455
H -4.213285 -1.720286 -2.863745
C -0.014341 -3.194058 -1.620841
H -0.821455 -3.588807 -0.983571
H -0.443098 -2.837894 -2.565648
H 0.715238 -3.991058 -1.838660
Cr 0.091261 0.271263 -1.876216

catalyst_model_B-12
Geometry with 61 atoms:
Total energy: -2960.233672790
P -1.912406 -0.429344 0.061813
P 1.547711 -0.214928 -0.173600
C 0.424808 -0.894827 -1.511376
C -0.941665 -0.189363 -1.521507
H 0.916746 -0.792980 -2.491688
H 0.298971 -1.971292 -1.310099
H -0.819155 0.898901 -1.632851
H -1.546579 -0.512718 -2.383018
C -3.153581 0.920634 -0.017385
C -4.428391 0.756751 -0.576907
C -2.805396 2.177529 0.533402
C -5.346989 1.809536 -0.597344
H -4.708331 -0.212569 -0.995644
C -3.724134 3.233594 0.515327
C -4.989064 3.042887 -0.051536
H -6.335752 1.664399 -1.037646
H -3.469699 4.204797 0.938255
H -5.698380 3.874102 -0.059713
C -2.866894 -1.979507 -0.159017
C -2.789319 -2.789791 -1.303617
C -3.674304 -2.395750 0.916918
C -3.512309 -3.986008 -1.372632
H -2.169333 -2.500817 -2.154345
C -4.405708 -3.581045 0.838566
H -3.735691 -1.782622 1.821139
C -4.323867 -4.381716 -0.307057
H -3.441944 -4.607567 -2.268787
H -5.036775 -3.886048 1.677053
H -4.889985 -5.314499 -0.365589
C 2.970910 -1.362904 -0.124648
C 3.128849 -2.468784 -0.971307
C 3.957428 -1.110041 0.861655
C 4.235436 -3.315652 -0.850270
H 2.389600 -2.676804 -1.746556
C 5.069477 -1.954010 0.980255
C 5.199181 -3.052844 0.124096
H 4.343765 -4.170949 -1.520453
H 5.835618 -1.763567 1.731640
H 6.069998 -3.705518 0.223803
C 2.212174 1.328760 -0.930429
C 3.464170 1.385687 -1.563437
C 1.425445 2.492702 -0.864761
C 3.917008 2.585421 -2.120245
H 4.091912 0.493489 -1.620818
C 1.875376 3.686716 -1.434328
H 0.454013 2.465504 -0.365831
C 3.124993 3.736561 -2.060082
H 4.895219 2.619464 -2.606598
H 1.250955 4.582521 -1.383366
H 3.482302 4.671607 -2.498462
O -1.544922 2.290719 1.069103
O 3.742606 -0.018433 1.636226
C -1.136175 3.533953 1.633551
H -0.104815 3.390639 1.982990
H -1.148739 4.340862 0.882186
H -1.772334 3.817320 2.488804
C 4.717436 0.379279 2.586432
H 5.686081 0.599347 2.105446
H 4.336708 1.297285 3.054352
H 4.864431 -0.387362 3.367429
Cr -0.079135 0.050178 1.762026

catalyst_model_B-13
Geometry with 61 atoms:
Total energy: -2960.232765090
P 1.593595 -0.335726 -0.394222
P -1.837917 -0.580701 -0.030161
C -0.600497 -0.512868 1.384914
C 0.744795 -1.175399 1.052431
H -0.453618 0.555095 1.610053
H -1.045827 -0.964661 2.285365
H 1.421877 -1.144183 1.917586
H 0.611539 -2.232586 0.771780
C 2.124884 1.279416 0.292583
C 1.655376 2.450982 -0.320693
C 2.952480 1.395809 1.439515
C 1.989828 3.716424 0.166674
H 1.010549 2.363362 -1.199581
C 3.297295 2.666698 1.925328
C 2.813669 3.813931 1.289577
H 1.614042 4.615113 -0.326734
H 3.936599 2.768166 2.801892
H 3.088597 4.795314 1.684338
C 3.100783 -1.339724 -0.690656
C 2.945850 -2.709749 -0.969440
C 4.383926 -0.772914 -0.750351
C 4.055670 -3.500953 -1.275122
H 1.952965 -3.169621 -0.952232
C 5.490720 -1.566087 -1.064760
H 4.525288 0.290977 -0.550008
C 5.332043 -2.931011 -1.323145
H 3.921560 -4.565824 -1.481710
H 6.484666 -1.113240 -1.105416
H 6.200150 -3.548501 -1.566462
C -2.745818 1.011427 0.124614
C -3.607225 1.257369 1.206092

C -2.556887 2.032179 -0.837263
C -4.273287 2.475473 1.343491
H -3.762376 0.470696 1.948683
C -3.228345 3.255536 -0.704534
C -4.079643 3.469571 0.382773
H -4.938096 2.645868 2.192810
H -3.100458 4.049851 -1.438526
H -4.594940 4.428937 0.472357
C -3.051746 -1.870608 0.448117
C -2.644016 -3.010573 1.163918
C -4.379033 -1.794600 -0.012945
C -3.550070 -4.042447 1.426421
H -1.616351 -3.106998 1.523563
C -5.280716 -2.826565 0.255094
H -4.714897 -0.918951 -0.574111
C -4.870103 -3.953270 0.975769
H -3.220741 -4.919614 1.989122
H -6.311437 -2.748624 -0.099977
H -5.577286 -4.759577 1.184588
O 3.367009 0.240410 2.001950
O -1.697371 1.781978 -1.889243
C 4.315726 0.257525 3.057486
H 5.251215 0.755554 2.749555
H 3.915513 0.754108 3.958380
H 4.530278 -0.793290 3.292644
C -1.490068 2.800918 -2.870300
H -0.770414 2.394409 -3.593468
H -2.426868 3.045253 -3.396565
H -1.066967 3.712358 -2.417941
Cr -0.317933 -0.222960 -2.037893

catalyst_model_B-14
Geometry with 61 atoms:
Total energy: -2960.229877790
P 1.771236 -0.053904 -0.529873
P -1.719625 0.034994 -0.481151
C -0.610617 0.524597 0.935923
C 0.693587 -0.285130 0.987567
H -0.404621 1.598355 0.788956
H -1.159970 0.440016 1.884360
H 1.286284 -0.013279 1.871534
H 0.479874 -1.362657 1.061541
C 2.613001 1.549972 -0.252548
C 2.498140 2.542467 -1.237809
C 3.355618 1.841812 0.921871
C 3.089862 3.798613 -1.086667
H 1.936311 2.319809 -2.149766
C 3.952723 3.102730 1.075257
C 3.814512 4.069567 0.075138
H 2.988396 4.554089 -1.868418
H 4.524657 3.337896 1.972594
H 4.284965 5.046548 0.212169
C 3.042504 -1.369616 -0.377584
C 2.616831 -2.708378 -0.304574
C 4.418206 -1.092766 -0.424046
C 3.549931 -3.746425 -0.249513
H 1.549796 -2.951443 -0.289941
C 5.348305 -2.134802 -0.376365
H 4.769860 -0.061408 -0.494399
C 4.919054 -3.462198 -0.283836
H 3.205226 -4.781462 -0.183358
H 6.416625 -1.905821 -0.408159
H 5.649442 -4.273976 -0.242760
C -3.157565 1.162945 -0.407126
C -3.469495 1.923401 -1.543173
C -3.991138 1.260777 0.734873
C -4.579950 2.770777 -1.568187
H -2.830624 1.839600 -2.427460
C -5.112429 2.103350 0.708359
C -5.396782 2.850878 -0.438752
H -4.808284 3.355469 -2.461661
H -5.765491 2.184001 1.577141
H -6.273241 3.503891 -0.442554
C -2.358243 -1.639668 -0.052719
C -2.920340 -2.396101 -1.096135
C -2.296948 -2.197514 1.234813
C -3.423578 -3.677218 -0.857025
H -2.971086 -1.976542 -2.106086
C -2.785817 -3.485610 1.469357
H -1.878144 -1.627403 2.064720
C -3.352997 -4.226174 0.427199
H -3.865878 -4.250012 -1.675907
H -2.729137 -3.910475 2.474798
H -3.737693 -5.231561 0.615345
O 3.448677 0.853194 1.837358
O -3.635143 0.513209 1.803135
C 4.268947 1.014303 2.984169
H 5.317337 1.214662 2.704371
H 3.902557 1.825124 3.637278
H 4.220080 0.063446 3.530933
C -4.480198 0.446588 2.940477
H -4.007829 -0.261710 3.634278
H -4.573513 1.427655 3.437550
H -5.484322 0.072873 2.676471
Cr -0.033115 -0.086263 -2.374409

catalyst_model_B-15
Geometry with 61 atoms:
Total energy: -2960.233012540
P -1.837045 -0.541437 0.059129
P 1.591368 0.089421 0.344984
C 0.767654 -0.743965 -1.126452
C -0.668543 -0.260903 -1.377262
H 1.387424 -0.578154 -2.017340
H 0.793869 -1.823940 -0.904603
H -0.683637 0.823387 -1.564172
H -1.082869 -0.727136 -2.285453
C -3.142780 0.720447 -0.219255
C -4.246418 0.498418 -1.055597
C -3.024670 1.970133 0.435636
C -5.220265 1.481793 -1.243736
H -4.346447 -0.464580 -1.561503
C -3.999984 2.957810 0.249572
C -5.091116 2.707396 -0.588910
H -6.072517 1.289950 -1.898963
H -3.923437 3.922307 0.749792
H -5.845772 3.485856 -0.725101
C -2.648642 -2.156173 -0.250916
C -3.774246 -2.493160 0.525305
C -2.134827 -3.105043 -1.150351
C -4.383927 -3.740154 0.386306
H -4.184911 -1.769508 1.235176
C -2.742644 -4.359062 -1.278170
H -1.257133 -2.881811 -1.760242
C -3.868159 -4.678703 -0.515559
H -5.264664 -3.982548 0.986308
H -2.333025 -5.086914 -1.983038
H -4.343279 -5.656971 -0.621125
C 3.088642 -0.903513 0.698978
C 3.342921 -1.226462 2.040939
C 3.987218 -1.370477 -0.293812
C 4.450899 -1.990512 2.413621
H 2.652607 -0.865269 2.809298
C 5.097821 -2.144525 0.077073
C 5.321545 -2.447900 1.423144
H 4.629917 -2.226412 3.464544
H 5.793968 -2.511592 -0.676792
H 6.192098 -3.050615 1.694200
C 2.141243 1.716194 -0.321708
C 3.471501 2.014731 -0.657979
C 1.162206 2.718698 -0.463520
C 3.808751 3.282687 -1.141014
H 4.251643 1.262081 -0.544391
C 1.500480 3.979256 -0.961486
H 0.128816 2.516667 -0.171601
C 2.826658 4.264745 -1.301282
H 4.848709 3.502585 -1.395553
H 0.727664 4.744073 -1.074363
H 3.095406 5.252696 -1.683179
O -1.922884 2.155498 1.239190
O 3.713521 -1.016749 -1.570041
C -1.715290 3.424242 1.858360
H -0.753197 3.358573 2.384117
H -1.656862 4.231532 1.110121
H -2.511908 3.651454 2.586087
C 4.589172 -1.392925 -2.620912
H 4.650191 -2.489747 -2.727462
H 4.165091 -0.966843 -3.539797
H 5.602935 -0.983276 -2.470253
Cr -0.361326 0.139832 1.996846

catalyst_model_B-16
Geometry with 61 atoms:
Total energy: -2960.229807150
P 1.676951 -0.202033 -0.399969
P -1.774489 -0.163746 -0.024379
C -0.565680 -0.673384 1.313952
C 0.776404 0.069262 1.213548
H -1.021398 -0.489233 2.300274
H -0.415981 -1.760947 1.213715
H 0.621450 1.158507 1.277400
H 1.438470 -0.196811 2.049241
C 2.937115 1.121145 -0.461994
C 2.939718 2.006466 -1.548862
C 3.920357 1.266612 0.548862
C 3.889953 3.025964 -1.652157
H 2.185385 1.886393 -2.332466
C 4.881497 2.283124 0.441014
C 4.857374 3.153402 -0.653613
H 3.877868 3.707841 -2.504908
H 5.646883 2.406683 1.206918
H 5.611090 3.942211 -0.720048
C 2.618955 -1.771081 -0.208183
C 2.518592 -2.613805 0.909673
C 3.439933 -2.156931 -1.282947
C 3.231324 -3.816795 0.950899
H 1.895733 -2.339923 1.763112
C 4.161353 -3.350877 -1.232643
H 3.525687 -1.512154 -2.162989
C 4.055410 -4.186869 -0.115471
H 3.145408 -4.465355 1.826498
H 4.805127 -3.632001 -2.069956
H 4.613771 -5.125417 -0.077822
C -3.274278 -1.150261 0.327475
C -3.344565 -2.170860 1.285944
C -4.418528 -0.872279 -0.461185
C -4.522779 -2.901926 1.471762
H -2.478194 -2.403951 1.907065
C -5.603299 -1.593765 -0.266568
C -5.645823 -2.606484 0.697944
H -4.561189 -3.692357 2.224309
H -6.490930 -1.375635 -0.860292
H -6.573339 -3.166155 0.841862
C -2.201343 1.555878 0.478778
C -3.231967 1.833242 1.391408
C -1.443860 2.618015 -0.042708
C -3.496087 3.150904 1.773670
H -3.835183 1.019269 1.800933
C -1.702514 3.934549 0.349575
H -0.641786 2.418245 -0.760127
C -2.731499 4.202752 1.257135
H -4.303277 3.357328 2.481129
H -1.102653 4.751597 -0.058934
H -2.939814 5.231762 1.560411
O 3.855791 0.391201 1.575186
O -4.267385 0.119044 -1.371267
C 4.870318 0.377915 2.567120
H 4.630767 -0.457351 3.238573
H 5.866299 0.206702 2.123879
H 4.884107 1.316274 3.148434
C -5.386934 0.582163 -2.108647
H -5.795690 -0.203318 -2.768188
H -6.185289 0.949459 -1.440996
H -5.027032 1.416501 -2.725564
Cr -0.241473 -0.393329 -2.058762

catalyst_model_B-17
Geometry with 61 atoms:
Total energy: -2960.230861910
P -1.739400 -0.025572 -0.045525
P 1.739422 0.025614 -0.045543
C 0.663805 -0.387631 -1.522669
C -0.663824 0.387618 -1.522688
H 1.224069 -0.174957 -2.446910
H 0.470533 -1.472328 -1.495696
H -0.470579 1.472319 -1.495805
H -1.224102 0.174863 -2.446901
C -3.164496 1.110979 -0.197609
C -3.274079 2.123064 -1.161668
C -4.197079 0.966162 0.762542
C -4.381289 2.977903 -1.182986
H -2.496299 2.250904 -1.916289
C -5.311520 1.814353 0.735954

C	-5.393758	2.817328	-0.236175
H	-4.451993	3.759538	-1.942344
H	-6.114525	1.701592	1.464365
H	-6.265337	3.476510	-0.248530
C	-2.397571	-1.686129	-0.492816
C	-3.565442	-1.848766	-1.255611
C	-1.683803	-2.824808	-0.082342
C	-4.005691	-3.128709	-1.602352
H	-4.136719	-0.974260	-1.576574
C	-2.120200	-4.103932	-0.439478
H	-0.778428	-2.717120	0.523478
C	-3.283941	-4.257324	-1.198719
H	-4.918305	-3.245380	-2.192356
H	-1.554465	-4.981723	-0.117179
H	-3.631451	-5.256561	-1.472573
C	3.164503	-1.110958	-0.197627
C	3.274086	-2.123018	-1.161710
C	4.197049	-0.966224	0.762579
C	4.381271	-2.977888	-1.183024
H	2.496326	-2.250805	-1.916362
C	5.311467	-1.814446	0.735996
C	5.393713	-2.817379	-0.236174
H	4.451976	-3.759497	-1.942410
H	6.114442	-1.701746	1.464450
H	6.265272	-3.476589	-0.248523
C	2.397596	1.686168	-0.492862
C	1.684053	2.824862	-0.082034
C	3.565280	1.848805	-1.255946
C	2.120454	4.103992	-0.439143
H	0.778867	2.717176	0.524068
C	4.005530	3.128752	-1.602672
H	4.136398	0.974292	-1.577171
C	3.283983	4.257378	-1.198709
H	1.554894	4.981793	-0.116565
H	4.917986	3.245417	-2.192921
H	3.631497	5.256620	-1.472543
O	-4.016509	-0.031451	1.660332
O	4.016458	0.031327	1.660433
C	-5.040134	-0.343637	2.591139
H	-4.680204	-1.206252	3.167974
H	-5.234817	0.495588	3.281703
H	-5.978715	-0.620965	2.081239
C	5.040047	0.343421	2.591309
H	5.978662	0.620746	2.081471
H	4.680120	1.206014	3.168179
H	5.234667	-0.495852	3.281834
Cr	0.000010	0.000058	1.832157

^{2}2A
Geometry with 65 atoms:
Total energy: -2889.242703790

Cr	0.115724	-0.628032	1.480595
P	1.567493	-0.083295	-0.334068
P	-1.583866	-0.246238	-0.238486
C	-0.714950	0.037393	-1.878307
C	0.690624	-0.569593	-1.902595
H	-1.336381	-0.346991	-2.700027
H	-0.652771	1.129624	-1.998997
H	0.648558	-1.667931	-1.941975
H	1.260366	-0.223102	-2.779030
C	3.186961	-0.924500	-0.354980
C	3.331601	-2.191547	-0.946158
C	4.279590	-0.352322	0.322122
C	4.551475	-2.869241	-0.868745
H	2.498381	-2.662376	-1.471650
C	5.496357	-1.033469	0.393880
H	4.186055	0.632575	0.784301
C	5.634924	-2.292538	-0.199992
H	4.654189	-3.851518	-1.336099
H	6.340994	-0.576833	0.915312
H	6.588114	-2.823470	-0.142687
C	1.886328	1.702037	-0.610144
C	2.911059	2.143160	-1.465449
C	1.024828	2.646244	-0.026083
C	3.071249	3.506859	-1.721850
H	3.590848	1.423306	-1.927646
C	1.182370	4.009122	-0.291475
H	0.213125	2.325818	0.631946
C	2.208117	4.440626	-1.137194
H	3.873932	3.842258	-2.383084
H	0.501910	4.731649	0.165194
H	2.336887	5.506334	-1.341661
C	-2.895705	-1.484523	-0.574561
C	-4.109284	-1.431545	0.132284
C	-2.661662	-2.551382	-1.458668
C	-5.073342	-2.426496	-0.049950
H	-4.312736	-0.606030	0.818811
C	-3.630639	-3.541571	-1.640278
H	-1.723171	-2.618907	-2.014234
C	-4.837024	-3.482300	-0.935768
H	-6.016316	-2.372218	0.499602
H	-3.440920	-4.363009	-2.335462
H	-5.593430	-4.257784	-1.078471
C	-2.513994	1.314720	0.053662
C	-3.177034	1.984995	-0.989537
C	-2.556026	1.856521	1.349233
C	-3.851428	3.181538	-0.739717
H	-3.170860	1.573796	-2.002171
C	-3.236300	3.052953	1.599055
H	-2.060516	1.346248	2.180379
C	-3.879999	3.718563	0.552977
H	-4.361156	3.697091	-1.557247
H	-3.262229	3.462719	2.611621
H	-4.409373	4.655181	0.744251
C	-0.204099	-2.680035	0.893357
C	0.802725	-2.547622	1.862604
H	-1.214991	-2.986860	1.185706
H	0.045281	-2.927326	-0.142997
H	1.860223	-2.623139	1.587572
H	0.587527	-2.768240	2.915142
C	0.541037	0.129570	3.388046
C	1.713502	0.337757	2.659287
H	-0.156136	0.967534	3.539981
H	0.443646	-0.691487	4.107014
H	2.562295	-0.345734	2.750345
H	1.959307	1.334365	2.279958

^{2}TS2-3A
Geometry with 65 atoms:
Total energy: -2889.200667870

Cr	0.056011	-0.525330	1.406713
P	1.560425	-0.127366	-0.423729
P	-1.483389	-0.168404	-0.421048
C	-0.625617	0.169489	-2.053426
C	0.745374	-0.506945	-2.057226
H	-1.255983	-0.163691	-2.890986
H	-0.515650	1.262474	-2.131893
H	0.649582	-1.600197	-2.147654
H	1.378879	-0.156823	-2.886704
C	3.057044	-1.186005	-0.367531
C	2.933852	-2.555233	-0.667292
C	4.287949	-0.698222	0.104297
C	4.026871	-3.413012	-0.520232
H	1.982597	-2.967354	-1.014619
C	5.378002	-1.560558	0.250326
H	4.401006	0.357199	0.359207
C	5.251808	-2.917247	-0.063039
H	3.919886	-4.472998	-0.763464
H	6.331394	-1.167793	0.612053
H	6.106286	-3.588624	0.050856
C	2.122670	1.600947	-0.685212
C	3.150611	1.915701	-1.592023
C	1.434973	2.641242	-0.040794
C	3.489459	3.248745	-1.833189
H	3.693661	1.119454	-2.106985
C	1.770133	3.975331	-0.289767
H	0.620765	2.414212	0.651367
C	2.800927	4.279586	-1.182715
H	4.294128	3.484803	-2.533785
H	1.223879	4.775607	0.215107
H	3.068512	5.321523	-1.374826
C	-2.764949	-1.417031	-0.825585
C	-4.071805	-1.322520	-0.320617
C	-2.398197	-2.548408	-1.576403
C	-4.998375	-2.338403	-0.575176
H	-4.374713	-0.450897	0.263373
C	-3.327981	-3.558868	-1.830417
H	-1.382852	-2.647979	-1.969887
C	-4.630265	-3.455921	-1.329259
H	-6.014720	-2.252293	-0.183066
H	-3.034861	-4.429900	-2.421740
H	-5.357190	-4.247090	-1.527914
C	-2.390703	1.380308	-0.050047
C	-3.222020	1.994858	-1.002001
C	-2.201651	1.997659	1.197412
C	-3.848445	3.207567	-0.706919
H	-3.383349	1.523245	-1.974870
C	-2.826420	3.213272	1.490940
H	-1.571850	1.524935	1.960704
C	-3.650731	3.817758	0.537455
H	-4.494977	3.679176	-1.450913
H	-2.673348	3.684693	2.464608
H	-4.143746	4.766071	0.764753
C	-1.619673	-1.390511	2.213999
C	-0.763086	-1.404767	3.383711
H	-2.558857	-0.826168	2.266707
H	-1.739774	-2.343402	1.678106
H	-0.281925	-2.367375	3.595705
H	-1.190938	-0.972313	4.294002
C	1.726790	0.001603	2.490499
C	0.790104	-0.232720	3.574549
H	2.586246	-0.676744	2.420386
H	1.997821	1.045117	2.282734
H	0.314973	0.670056	3.980740
H	1.145405	-0.878639	4.383532

^{4}2A
Geometry with 65 atoms:
Total energy: -2889.288231630

Cr	0.050982	-0.512019	1.486131
P	1.627646	0.091271	-0.368747
P	-1.520174	-0.085050	-0.345699
C	-0.645267	0.318420	-1.958154
C	0.794295	-0.201311	-2.005759
H	-1.241568	-0.043680	-2.810402
H	-0.647454	1.418704	-2.007365
H	0.834114	-1.285835	-2.188728
H	1.369134	0.278936	-2.812404
C	3.306507	-0.619291	-0.541284
C	3.444554	-1.954473	-0.966174
C	4.449647	0.092849	-0.139697
C	4.703631	-2.557235	-1.003937
H	2.570102	-2.535635	-1.271259
C	5.707071	-0.517323	-0.175622
H	4.364173	1.127511	0.199389
C	5.837553	-1.840266	-0.607594
H	4.798777	-3.591973	-1.341923
H	6.589614	0.047550	0.134569
H	6.821937	-2.313472	-0.634982
C	1.827392	1.910549	-0.286089
C	2.344769	2.664744	-1.353458
C	1.420440	2.568855	0.886991
C	2.444829	4.053441	-1.244575
H	2.677893	2.170457	-2.269805
C	1.521702	3.958597	0.995342
H	1.019145	1.986368	1.724700
C	2.032678	4.700713	-0.073220
H	2.848094	4.634993	-2.077062
H	1.202278	4.460126	1.911933
H	2.112737	5.787569	0.006094
C	-2.356855	-1.696195	-0.629638
C	-3.491866	-2.037572	0.130350
C	-1.826991	-2.645946	-1.521012
C	-4.081726	-3.295839	-0.004581
H	-3.930746	-1.311108	0.817437
C	-2.417423	-3.907140	-1.648074
H	-0.954724	-2.412851	-2.133461
C	-3.544157	-4.236113	-0.890232
H	-4.969227	-3.541410	0.583767
H	-1.996786	-4.632009	-2.349425
H	-4.006972	-5.220426	-0.993693
C	-2.833495	1.191878	-0.309113
C	-4.043633	1.054863	-1.009494
C	-2.565748	2.387137	0.379976
C	-4.974573	2.097228	-1.007987
H	-4.265889	0.134991	-1.555082
C	-3.495576	3.429579	0.371512
H	-1.622716	2.507752	0.920014
C	-4.703176	3.283574	-0.318664
H	-5.915922	1.982013	-1.550931
H	-3.278299	4.355669	0.909354
H	-5.434398	4.095694	-0.319456
C	1.018707	-2.783639	1.729955

C	1.955406	-2.105477	2.425604
H	0.143190	-3.224714	2.218204
H	1.162298	-3.021652	0.670456
H	2.875097	-1.757016	1.945629
H	1.870082	-1.953066	3.504947
C	-1.719625	-0.256405	2.714964
C	-0.567940	-0.482648	3.498321
H	-2.145846	0.747527	2.620407
H	-2.445581	-1.065142	2.579929
H	-0.422724	-1.446978	3.998419
H	-0.062258	0.362917	3.988344

^{4}TS2-3A
Geometry with 65 atoms:
Total energy: -2889.278236010

Cr	0.068313	-0.661032	1.471639
P	1.635181	-0.154279	-0.385442
P	-1.501513	-0.183368	-0.417460
C	-0.580648	0.122052	-2.022441
C	0.793038	-0.555526	-1.998993
H	-1.185407	-0.225135	-2.873153
H	-0.466926	1.213018	-2.116577
H	0.691719	-1.651021	-2.057711
H	1.419338	-0.231415	-2.844978
C	3.241370	-1.028112	-0.426810
C	3.391872	-2.242610	-1.118690
C	4.324845	-0.523804	0.316518
C	4.606592	-2.933323	-1.074123
H	2.569536	-2.660862	-1.703040
C	5.535927	-1.217278	0.355528
H	4.227238	0.419585	0.857817
C	5.679810	-2.423361	-0.338595
H	4.713407	-3.873032	-1.621452
H	6.372156	-0.811518	0.930021
H	6.628867	-2.963861	-0.307733
C	2.009314	1.632851	-0.563999
C	3.052135	2.083209	-1.392652
C	1.179042	2.572437	0.069252
C	3.258804	3.452154	-1.576427
H	3.710400	1.365868	-1.888790
C	1.383059	3.941420	-0.124253
H	0.359206	2.241460	0.711030
C	2.424827	4.382201	-0.945018
H	4.075069	3.794849	-2.216995
H	0.726889	4.661897	0.369808
H	2.589968	5.452282	-1.092778
C	-2.740229	-1.469916	-0.828169
C	-4.063939	-1.375736	-0.369879
C	-2.334505	-2.617665	-1.532179
C	-4.969235	-2.410674	-0.623242
H	-4.396239	-0.490634	0.176778
C	-3.244030	-3.646799	-1.785265
H	-1.306329	-2.716952	-1.890316
C	-4.563122	-3.545814	-1.330069
H	-5.998811	-2.325646	-0.267147
H	-2.921229	-4.531430	-2.339714
H	-5.273465	-4.352199	-1.527434
C	-2.457639	1.350980	-0.122899
C	-3.124452	2.001177	-1.176438
C	-2.509730	1.901612	1.168175
C	-3.822980	3.186312	-0.938430
H	-3.101662	1.582502	-2.185657
C	-3.212017	3.087468	1.403852
H	-2.004084	1.402467	1.998971
C	-3.866741	3.731176	0.350313
H	-4.337961	3.686669	-1.762048
H	-3.247424	3.506749	2.412173
H	-4.414920	4.658697	0.532758
C	-1.577646	-1.660931	2.215350
C	-0.746975	-1.673301	3.407457
H	-2.535152	-1.128469	2.270357
H	-1.652049	-2.592444	1.637894
H	-0.204586	-2.610622	3.581530
H	-1.224492	-1.319515	4.326768
C	1.672699	-0.071589	2.640962
C	0.728636	-0.419962	3.691168
H	2.571310	-0.695601	2.558324
H	1.873775	0.994618	2.475973
H	0.179055	0.429488	4.116560
H	1.109782	-1.072202	4.482941

^{6}2A
Geometry with 65 atoms:
Total energy: -2889.321313180

Cr	0.009004	-0.215780	1.620061
P	1.699212	0.055824	-0.264569
P	-1.673829	-0.031764	-0.285742
C	-0.652796	0.416093	-1.782615
C	0.709454	-0.290584	-1.812111
H	-1.225171	0.217823	-2.702520
H	-0.523279	1.508993	-1.729322
H	0.583917	-1.384411	-1.864569
H	1.281702	0.025548	-2.698481
C	3.161296	-1.039755	-0.368103
C	3.541166	-1.728503	-1.532262
C	3.935951	-1.184639	0.797890
C	4.674956	-2.547775	-1.525593
H	2.964937	-1.630600	-2.454177
C	5.072762	-1.994859	0.797530
H	3.648926	-0.654575	1.711025
C	5.441927	-2.681071	-0.364746
H	4.961703	-3.080823	-2.435496
H	5.669059	-2.095492	1.707660
H	6.327765	-3.320852	-0.364574
C	2.346270	1.754359	-0.561915
C	3.572038	1.996199	-1.204246
C	1.562400	2.846608	-0.149468
C	3.997944	3.307702	-1.433016
H	4.200335	1.161246	-1.523112
C	1.985754	4.156380	-0.389055
H	0.612812	2.674076	0.364144
C	3.206752	4.388413	-1.029736
H	4.955064	3.485926	-1.929571
H	1.365099	4.996472	-0.067547
H	3.544483	5.411889	-1.209991
C	-2.481414	-1.629512	-0.691859
C	-3.305991	-2.202826	0.295369
C	-2.281899	-2.319896	-1.897885
C	-3.927628	-3.432029	0.074003
H	-3.468839	-1.678518	1.241891
C	-2.896617	-3.559203	-2.111419
H	-1.649878	-1.901892	-2.683577
C	-3.720376	-4.115753	-1.130235
H	-4.573162	-3.861072	0.844312
H	-2.732630	-4.087547	-3.053874
H	-4.201479	-5.081757	-1.301575
C	-3.023294	1.212308	-0.312140
C	-4.222744	1.016529	-1.016545
C	-2.824264	2.415689	0.387364
C	-5.202124	2.013661	-1.022165
H	-4.397636	0.083424	-1.557305
C	-3.801375	3.414026	0.371415
H	-1.899498	2.575019	0.950087
C	-4.993352	3.212218	-0.331963
H	-6.134039	1.852620	-1.569807
H	-3.635938	4.346882	0.916050
H	-5.762662	3.988310	-0.338362
C	-0.419349	-2.541339	2.484462
C	0.857209	-2.230567	2.812926
H	-1.246025	-2.389974	3.186567
H	-0.665177	-3.051308	1.547112
H	1.696575	-2.488902	2.158387
H	1.112112	-1.826922	3.798744
C	-0.846472	0.975731	3.577033
C	0.439192	1.393143	3.433951
H	-1.682930	1.528433	3.136260
H	-1.107314	0.153705	4.251835
H	1.259592	0.920789	3.984357
H	0.692474	2.296818	2.869452

^{6}TS2-3A
Geometry with 65 atoms:
Total energy: -2889.251049020

Cr	0.082973	-0.206762	1.553000
P	-1.697891	-0.118245	-0.373867
P	1.599947	-0.153150	-0.453970
C	0.567077	0.161998	-1.976941
C	-0.757011	-0.607713	-1.906668
H	0.380771	1.244951	-2.041741
H	1.146301	-0.122068	-2.868769
H	-1.369504	-0.417277	-2.802029
H	-0.572302	-1.693275	-1.850608
C	-2.262194	1.585930	-0.763743
C	-1.627397	2.675877	-0.143990
C	-3.286161	1.825055	-1.696896
C	-2.000556	3.986296	-0.459637
H	-0.840664	2.505684	0.597259
C	-3.659263	3.134347	-2.006971
H	-3.799861	0.987069	-2.175200
C	-3.016610	4.215365	-1.391435
H	-1.502577	4.826717	0.029920
H	-4.458671	3.313030	-2.730294
H	-3.314439	5.238211	-1.634633
C	-3.216871	-1.137227	-0.355219
C	-4.184876	-0.840764	0.624024
C	-3.432404	-2.217823	-1.227041
C	-5.346807	-1.606778	0.722780
H	-4.033786	-0.000963	1.307954
C	-4.597332	-2.985278	-1.119371
H	-2.705627	-2.471947	-2.000628
C	-5.554368	-2.683203	-0.147613
H	-6.092837	-1.363669	1.483184
H	-4.756392	-3.821484	-1.804717
H	-6.463069	-3.284700	-0.068121
C	2.808147	1.220585	-0.375944
C	2.368294	2.543339	-0.570572
C	4.136946	0.990086	0.019802
C	3.251037	3.611609	-0.397437
H	1.334449	2.752955	-0.857198
C	5.014492	2.064120	0.193077
H	4.492186	-0.028039	0.191509
C	4.575975	3.374697	-0.016935
H	2.900685	4.633836	-0.560148
H	6.047267	1.873080	0.494406
H	5.265332	4.211619	0.117704
C	2.536094	-1.672839	-0.850957
C	3.460796	-1.693764	-1.911771
C	2.301932	-2.845602	-0.115372
C	4.141262	-2.871275	-2.223537
H	3.658123	-0.785212	-2.486842
C	2.982095	-4.025275	-0.434820
H	1.589345	-2.840914	0.713700
C	3.902280	-4.037622	-1.485971
H	4.862268	-2.879928	-3.044603
H	2.794469	-4.933845	0.142173
H	4.437895	-4.957652	-1.732638
C	-1.581452	0.073439	3.194946
C	-0.925203	-0.031408	4.412542
H	-1.868046	1.061445	2.813848
H	-2.148572	-0.783321	2.810292
H	-0.967799	-0.964354	4.978769
H	-0.688659	0.866940	4.986911
C	1.788206	-0.388301	2.884061
C	1.390533	-0.388556	4.259155
H	2.200824	-1.338481	2.507132
H	2.393437	0.472759	2.558931
H	1.578930	0.492287	4.879757
H	1.318354	-1.336136	4.800996

^{2}2B
Geometry with 73 atoms:
Total energy: -3118.329193560

Cr	0.017117	0.396913	1.477232
P	-1.611121	0.085356	-0.266600
P	1.556337	-0.248668	-0.375733
C	0.634950	0.083964	-1.961214
C	-0.807334	-0.429365	-1.884290
H	0.640514	1.177847	-2.091571
H	1.170043	-0.357952	-2.815177
H	-1.393427	-0.027492	-2.724124
H	-0.837949	-1.524645	-1.933711
C	-2.061157	1.820266	-0.697302
C	-3.236773	2.196029	-1.356413
C	-1.127575	2.817600	-0.354717
C	-3.479656	3.534014	-1.682241
H	-3.976129	1.433762	-1.611689
C	-1.354403	4.156445	-0.683496
C	-2.535061	4.505291	-1.350328
H	-4.403856	3.813365	-2.192470
H	-0.637704	4.934332	-0.424483
H	-2.712036	5.553650	-1.601710
C	-3.164163	-0.883060	-0.233112
C	-3.818635	-1.292225	-1.410886

C	-3.695090	-1.266089	1.010107
C	-4.983901	-2.059848	-1.339665
H	-3.426589	-1.019042	-2.392375
C	-4.861711	-2.032401	1.077105
H	-3.186153	-0.973145	1.927523
C	-5.508120	-2.430154	-0.096785
H	-5.484487	-2.370168	-2.260193
H	-5.263577	-2.323076	2.050726
H	-6.418964	-3.031627	-0.044648
C	2.294942	-1.925446	-0.550200
C	3.672584	-2.114477	-0.734972
C	1.460089	-3.065147	-0.454966
C	4.220539	-3.397263	-0.824211
H	4.331935	-1.248055	-0.808009
C	2.008241	-4.351900	-0.539140
C	3.385122	-4.509929	-0.723220
H	5.295500	-3.521516	-0.970289
H	1.371091	-5.232502	-0.462283
H	3.801650	-5.518152	-0.787568
C	3.009764	0.867411	-0.381063
C	3.429779	1.605221	-1.498570
C	3.701493	1.014083	0.837239
C	4.513858	2.484034	-1.394229
H	2.924338	1.500216	-2.460556
C	4.786885	1.886589	0.935909
H	3.391412	0.438313	1.714729
C	5.190944	2.628745	-0.179932
H	4.833246	3.053813	-2.270380
H	5.316933	1.990002	1.885832
H	6.037130	3.315859	-0.103579
O	0.005156	2.394518	0.333527
O	0.135571	-2.822177	-0.285878
C	0.999241	3.374030	0.670818
H	1.803408	2.843475	1.190498
H	1.410268	3.834723	-0.239511
H	0.576373	4.146428	1.331146
C	-0.786272	-3.901221	-0.212218
H	-0.586185	-4.543406	0.661837
H	-1.781360	-3.449397	-0.106699
H	-0.764668	-4.512557	-1.130423
C	-0.439408	1.533099	3.225738
C	-1.671131	1.384895	2.582958
H	-0.206280	0.951983	4.123663
H	0.129155	2.466328	3.127847
H	-2.085301	2.195181	1.978007
H	-2.414471	0.685950	2.972678
C	0.880559	-1.201391	2.616537
C	-0.494599	-1.434884	2.508505
H	1.592468	-1.809708	2.053092
H	1.289305	-0.727758	3.517243
H	-1.164805	-1.178216	3.332824
H	-0.869698	-2.203252	1.833561

^{2}TS2-3B
Geometry with 73 atoms:
Total energy: -3118.326412220

Cr	-0.000010	-0.000109	1.234288
P	1.471190	-0.052003	-0.615154
P	-1.471208	0.052073	-0.615151
O	0.501492	-2.276562	1.140757
O	-0.501472	2.276365	1.141099
C	-0.699340	-0.304193	-2.275704
C	0.699325	0.304500	-2.275656
H	-0.649498	-1.399017	-2.383511
H	-1.329788	0.083555	-3.089865
H	1.329777	-0.083125	-3.089872
H	0.649478	1.399341	-2.383292
C	1.901504	-1.831882	-0.749167
C	2.734294	-2.307564	-1.774822
C	1.328224	-2.760559	0.148484
C	3.009672	-3.667685	-1.914296
H	3.181900	-1.592311	-2.469625
C	1.599892	-4.129906	0.009775
C	2.437167	-4.572325	-1.017360
H	3.664139	-4.018074	-2.714975
H	1.166151	-4.861486	0.689375
H	2.639431	-5.641942	-1.112116
C	3.046535	0.884329	-0.650647
C	2.993576	2.263231	-0.928313
C	4.275635	0.305589	-0.295972
C	4.152885	3.039894	-0.873397
H	2.044768	2.742339	-1.186789
C	5.433100	1.088021	-0.239109
H	4.335586	-0.759475	-0.064025
C	5.375906	2.453755	-0.529393
H	4.101093	4.107894	-1.099723
H	6.384499	0.624780	0.033829
H	6.282496	3.062306	-0.486676
C	-1.901477	1.831985	-0.748905
C	-2.734236	2.307840	-1.774505
C	-1.328181	2.760521	0.148883
C	-3.009574	3.667988	-1.913792
H	-3.181849	1.592699	-2.469419
C	-1.599808	4.129895	0.010362
C	-2.437056	4.572485	-1.016721
H	-3.664018	4.018507	-2.714433
H	-1.166055	4.861366	0.690072
H	-2.639289	5.642120	-1.111328
C	-3.046577	-0.884213	-0.650786
C	-2.993653	-2.263079	-0.928635
C	-4.275666	-0.305488	-0.296045
C	-4.152984	-3.039717	-0.873836
H	-2.044856	-2.742180	-1.187162
C	-5.433152	-1.087896	-0.239297
H	-4.335590	0.759546	-0.063956
C	-5.375993	-2.453592	-0.529765
H	-4.101219	-4.107689	-1.100303
H	-6.384541	-0.624666	0.033695
H	-6.282600	-3.062125	-0.487137
C	-0.026988	-3.196376	2.102443
H	-0.601181	-2.607480	2.822484
H	-0.697940	-3.923621	1.618921
H	0.785798	-3.720632	2.628650
C	0.027058	3.196044	2.102889
H	-0.785699	3.720277	2.629163
H	0.601231	2.607039	2.822858
H	0.698039	3.923315	1.619444
C	-1.822644	-0.202834	2.238174
C	-1.000992	0.045222	3.410466
H	-2.536650	0.586439	1.973314
H	-2.258262	-1.203715	2.125379
H	-1.028827	-0.719616	4.193077
H	-1.102874	1.048652	3.837353
C	1.822622	0.202451	2.238217
C	1.000962	-0.045788	3.410464
H	2.536621	-0.586785	1.973232
H	2.258254	1.203344	2.125589
H	1.028793	0.718927	4.193196
H	1.102835	-1.049286	3.837195

^{4}2B
Geometry with 73 atoms:
Total energy: -3118.366693530

Cr	0.067866	-0.211765	1.550195
P	-1.545569	0.151491	-0.374997
P	1.647878	0.039315	-0.343987
O	-0.285414	2.788286	-0.091596
O	0.163276	-2.352722	0.541254
C	0.786446	0.532172	-1.926129
C	-0.600196	-0.114496	-1.965590
H	0.698149	1.626026	-1.939938
H	1.389008	0.221847	-2.794036
H	-1.187201	0.261186	-2.816982
H	-0.504224	-1.206655	-2.078044
C	-2.364504	1.788984	-0.577692
C	-3.727093	1.911950	-0.886585
C	-1.600144	2.967300	-0.396278
C	-4.327404	3.167571	-1.019074
H	-4.330674	1.013157	-1.025394
C	-2.198753	4.226382	-0.531299
C	-3.559388	4.318638	-0.841824
H	-5.389658	3.241172	-1.261153
H	-1.615011	5.136859	-0.397479
H	-4.016390	5.305824	-0.945173
C	-2.928475	-1.055165	-0.470502
C	-3.310862	-1.690790	-1.664172
C	-3.620276	-1.366302	0.714842
C	-4.352149	-2.624753	-1.666133
H	-2.807299	-1.464010	-2.605370
C	-4.666476	-2.291063	0.708619
H	-3.336816	-0.887772	1.654548
C	-5.031367	-2.927028	-0.482548
H	-4.636132	-3.114193	-2.601030
H	-5.194232	-2.519732	1.637797
H	-5.845714	-3.655670	-0.488294
C	2.083885	-1.712445	-0.712825
C	3.197841	-2.064899	-1.487470
C	1.251307	-2.738686	-0.216571
C	3.488959	-3.401976	-1.767569
H	3.852435	-1.277350	-1.868436
C	1.534972	-4.080788	-0.495172
C	2.653598	-4.403207	-1.270059
H	4.363424	-3.658216	-2.369340
H	0.899961	-4.880633	-0.116966
H	2.868502	-5.453760	-1.479921
C	3.246348	0.935584	-0.371760
C	3.456616	2.056991	-1.193875
C	4.278504	0.527544	0.495567
C	4.668145	2.754860	-1.145803
H	2.682385	2.399156	-1.881931
C	5.487343	1.223947	0.535398
H	4.146328	-0.347801	1.132643
C	5.685301	2.342094	-0.282213
H	4.816568	3.621993	-1.794184
H	6.280282	0.889390	1.208775
H	6.632115	2.886483	-0.248767
C	0.565326	3.908770	0.103952
H	1.549320	3.503606	0.372198
H	0.658547	4.508764	-0.817467
H	0.206411	4.556364	0.922181
C	-0.732500	-3.357852	1.029253
H	-0.210338	-4.061098	1.696389
H	-1.512146	-2.832957	1.590717
H	-1.199367	-3.901280	0.193262
C	-0.584745	1.698169	2.931886
C	-1.711958	0.946353	2.967142
H	0.213112	1.580236	3.669921
H	-0.499832	2.543583	2.247534
H	-2.561347	1.189151	2.322766
H	-1.862719	0.166740	3.719507
C	1.850520	-0.759144	2.625056
C	0.686283	-1.131519	3.342161
H	2.447998	-1.529131	2.125734
H	2.425619	0.121490	2.935258
H	0.391907	-0.587661	4.246768
H	0.370104	-2.182534	3.340329

^{4}TS2-3B
Geometry with 73 atoms:
Total energy: -3118.363816240

Cr	-0.000010	-0.000082	1.425369
P	1.522529	-0.122697	-0.530412
P	-1.522532	0.122760	-0.530409
O	0.193465	-2.466274	0.748085
O	-0.193415	2.466156	0.748367
C	-0.698244	-0.309966	-2.148047
C	0.698252	0.310249	-2.147996
H	-0.631788	-1.407289	-2.214767
H	-1.310354	0.043400	-2.991982
H	1.310371	-0.042995	-2.991975
H	0.631788	1.407580	-2.214561
C	1.930105	-1.896898	-0.771998
C	2.931662	-2.298454	-1.670229
C	1.193044	-2.890231	-0.084715
C	3.223322	-3.647565	-1.875334
H	3.500168	-1.536786	-2.209353
C	1.489365	-4.246833	-0.283496
C	2.500820	-4.615437	-1.174109
H	4.009605	-3.939340	-2.574415
H	0.938053	-5.021772	0.247462
H	2.720428	-5.676135	-1.318613
C	3.108815	0.790117	-0.547887
C	3.126759	2.132288	-0.970244
C	4.282407	0.228944	-0.014101
C	4.298984	2.887406	-0.879182
H	2.226751	2.602341	-1.372517
C	5.451783	0.988419	0.074659
H	4.288299	-0.805590	0.334045
C	5.464686	2.317778	-0.358236
H	4.300378	3.925739	-1.220036
H	6.357754	0.536625	0.485983
H	6.381129	2.908789	-0.289504
C	-1.930112	1.896997	-0.771737

C	-2.931693	2.298690	-1.669881
C	-1.193035	2.890231	-0.084326
C	-3.223369	3.647832	-1.874764
H	-3.500203	1.537107	-2.209119
C	-1.489376	4.246861	-0.282878
C	-2.500861	4.615599	-1.173402
H	-4.009671	3.939710	-2.573780
H	-0.938055	5.021719	0.248190
H	-2.720483	5.676318	-1.317728
C	-3.108813	-0.790063	-0.548003
C	-3.126737	-2.132189	-0.970502
C	-4.282416	-0.228960	-0.014168
C	-4.298956	-2.887328	-0.879538
H	-2.226721	-2.602193	-1.372814
C	-5.451786	-0.988457	0.074495
H	-4.288320	0.805535	0.334092
C	-5.464671	-2.317769	-0.358546
H	-4.300335	-3.925625	-1.220503
H	-6.357766	-0.536717	0.485859
H	-6.381109	-2.908795	-0.289891
C	-0.588950	-3.422932	1.459009
H	-1.348592	-2.854194	2.008014
H	-1.096817	-4.117322	0.770969
H	0.029359	-3.991826	2.172813
C	0.589056	3.422715	1.459364
H	-0.029193	3.991494	2.173311
H	1.348756	2.853902	2.008210
H	1.096850	4.117215	0.771381
C	-1.840158	-0.003452	2.410761
C	-0.970236	-0.209879	3.548365
H	-2.361261	0.961011	2.348291
H	-2.466709	-0.847967	2.104741
H	-0.912404	-1.247662	3.898316
H	-1.086940	0.482829	4.387544
C	1.840125	0.003181	2.410788
C	0.970188	0.209511	3.548398
H	2.361215	-0.961283	2.348230
H	2.466690	0.847718	2.104856
H	0.912355	1.247265	3.898439
H	1.086877	-0.483271	4.387518

^{6}2B
Geometry with 73 atoms:
Total energy: -3118.393763650

Cr	-0.003093	-0.005030	1.563317
P	-1.668670	0.127365	-0.336161
P	1.654829	-0.119353	-0.351555
O	-0.281617	2.686180	-0.166625
O	0.274350	-2.681643	-0.225068
C	0.706620	0.271657	-1.917140
C	-0.734419	-0.255071	-1.912565
H	0.708859	1.368143	-1.991827
H	1.249171	-0.130603	-2.786436
H	-1.284871	0.155039	-2.773214
H	-0.737824	-1.350678	-1.996046
C	-2.413793	1.788177	-0.622244
C	-3.768399	1.973818	-0.930753
C	-1.588126	2.928911	-0.472446
C	-4.302298	3.256019	-1.094809
H	-4.419294	1.104138	-1.040720
C	-2.120021	4.214214	-0.635126
C	-3.475166	4.369544	-0.946844
H	-5.360100	3.379598	-1.336464
H	-1.489780	5.096082	-0.523000
H	-3.880590	5.376514	-1.072682
C	-3.098466	-1.020286	-0.367440
C	-3.586609	-1.624023	-1.538950
C	-3.711733	-1.321635	0.862209
C	-4.661040	-2.516827	-1.476569
H	-3.136432	-1.402903	-2.508730
C	-4.792608	-2.204624	0.920426
H	-3.337791	-0.862731	1.782386
C	-5.265654	-2.808000	-0.249702
H	-5.030286	-2.983854	-2.393000
H	-5.262858	-2.426638	1.881590
H	-6.106163	-3.504974	-0.205586
C	2.408786	-1.774803	-0.645690
C	3.768995	-1.954559	-0.932348
C	1.585695	-2.919412	-0.512309
C	4.310631	-3.234459	-1.089528
H	4.418301	-1.082237	-1.029587
C	2.125023	-4.202364	-0.668106
C	3.485939	-4.351695	-0.956975
H	5.372871	-3.353336	-1.313449
H	1.496466	-5.086860	-0.567789
H	3.897701	-5.356810	-1.076918
C	3.079801	1.034326	-0.385138
C	3.557626	1.646082	-1.556668
C	3.701416	1.330463	0.841627
C	4.629398	2.542218	-1.497189
H	3.101895	1.428112	-2.524550
C	4.779622	2.216996	0.896899
H	3.336436	0.864446	1.761697
C	5.241906	2.828770	-0.273179
H	4.990607	3.015137	-2.413813
H	5.256307	2.435102	1.855789
H	6.080374	3.528337	-0.231349
C	0.623434	3.767529	0.003412
H	1.599922	3.320732	0.227798
H	0.712200	4.367677	-0.918082
H	0.319712	4.422947	0.837322
C	-0.629583	-3.766102	-0.070329
H	-0.335559	-4.422887	0.765924
H	-1.610033	-3.321902	0.142122
H	-0.703629	-4.364442	-0.994284
C	0.654208	1.774436	3.172920
C	-0.702360	1.792297	3.114532
H	1.185256	1.257695	3.978953
H	1.263842	2.376392	2.492119
H	-1.235678	2.407240	2.382706
H	-1.313474	1.293440	3.873813
C	0.784956	-1.876947	3.029622
C	-0.568459	-1.882818	3.113096
H	1.316380	-2.453774	2.266302
H	1.401257	-1.390176	3.792361
H	-1.090719	-1.399028	3.945065
H	-1.184393	-2.469678	2.425106

^{6}TS2-3B
Geometry with 73 atoms:
Total energy: -3118.333194250

Cr	0.078016	0.015693	1.489611
P	1.621281	-0.135944	-0.495238
P	-1.636252	0.137912	-0.476237
O	0.062463	-2.522226	0.226348
O	-0.115627	2.553181	0.217768
C	-0.711841	-0.312396	-2.029155
C	0.678004	0.330701	-2.030540
H	-0.623497	-1.408890	-2.046592
H	-1.289275	-0.001788	-2.913545
H	1.252675	0.030388	-2.920316
H	0.590148	1.427232	-2.034251
C	2.104951	-1.885068	-0.789136
C	3.307643	-2.236312	-1.419694
C	1.232314	-2.914922	-0.360127
C	3.653061	-3.574916	-1.619484
H	3.988326	-1.449628	-1.752676
C	1.580134	-4.258148	-0.554004
C	2.787599	-4.578902	-1.181655
H	4.593837	-3.829427	-2.111917
H	0.919909	-5.057868	-0.220020
H	3.048231	-5.630174	-1.326767
C	3.176260	0.823714	-0.552113
C	3.382402	1.882326	-1.453056
C	4.171812	0.531832	0.400499
C	4.560643	2.634450	-1.398584
H	2.634818	2.132335	-2.207263
C	5.347589	1.282086	0.446238
H	4.031170	-0.290006	1.105750
C	5.543477	2.338097	-0.450978
H	4.710303	3.452948	-2.107060
H	6.113687	1.041618	1.187237
H	6.463435	2.926460	-0.412885
C	-2.156214	1.877751	-0.776583
C	-3.371024	2.207268	-1.395421
C	-1.295588	2.924332	-0.363764
C	-3.738285	3.539337	-1.601759
H	-4.043301	1.407703	-1.715065
C	-1.662891	4.260997	-0.566872
C	-2.881796	4.559358	-1.183967
H	-4.688340	3.776312	-2.085168
H	-1.009389	5.072715	-0.248423
H	-3.158447	5.605493	-1.336403
C	-3.180792	-0.841845	-0.518978
C	-3.407967	-1.873576	-1.445595
C	-4.142677	-0.599829	0.481448
C	-4.569870	-2.649214	-1.367445
H	-2.688810	-2.084144	-2.238662
C	-5.303496	-1.371130	0.550358
H	-3.987588	0.201866	1.207529
C	-5.517879	-2.402387	-0.371524
H	-4.734417	-3.447531	-2.095461
H	-6.042558	-1.167947	1.329164
H	-6.424728	-3.009263	-0.314646
C	-0.870395	-3.498208	0.678821
H	-1.722921	-2.943010	1.089612
H	-1.225928	-4.128839	-0.152457
H	-0.434562	-4.134179	1.467341
C	0.823214	3.543151	0.624519
H	0.404841	4.195353	1.409297
H	1.688210	3.000900	1.027029
H	1.153697	4.157400	-0.229320
C	-1.690909	0.060981	3.056883
C	-1.102498	0.067663	4.308710
H	-2.056756	0.999986	2.623697
H	-2.114450	-0.866476	2.654778
H	-1.054729	-0.849332	4.899945
H	-1.003651	1.002224	4.864846
C	1.722081	-0.004440	2.925619
C	1.267435	0.009273	4.281725
H	2.222151	-0.931310	2.600195
H	2.265733	0.893700	2.592801
H	1.319383	0.933809	4.864311
H	1.273294	-0.914562	4.867594

^{4}TS5-6A-01
Geometry with 71 atoms:
Total energy: -2967.017803000

Cr	-0.016021	-0.057269	1.290493
P	-1.581017	0.425961	-0.596658
P	1.584785	0.411283	-0.553085
C	0.721910	0.654805	-2.199299
C	-0.690438	1.222273	-2.031610
H	1.337229	1.289530	-2.855572
H	0.684401	-0.341552	-2.664696
H	-0.666189	2.298263	-1.794279
H	-1.275458	1.104009	-2.956378
C	-3.012275	1.526511	-0.303672
C	-3.795248	2.010939	-1.368564
C	-3.317184	1.923306	1.009029
C	-4.865637	2.871844	-1.118134
H	-3.578061	1.713216	-2.397102
C	-4.390540	2.784448	1.255264
H	-2.716653	1.556878	1.844425
C	-5.165586	3.257899	0.193334
H	-5.469219	3.242314	-1.950275
H	-4.619689	3.085705	2.280203
H	-6.004538	3.931030	0.386112
C	-2.240740	-1.160431	-1.256630
C	-3.615173	-1.403662	-1.411161
C	-1.327437	-2.195854	-1.540088
C	-4.063868	-2.650020	-1.860843
H	-4.343758	-0.625605	-1.177685
C	-1.780740	-3.435213	-1.995740
H	-0.253318	-2.049901	-1.400552
C	-3.151186	-3.665080	-2.157895
H	-5.136167	-2.826140	-1.976271
H	-1.060184	-4.226319	-2.217178
H	-3.506320	-4.637044	-2.508627
C	2.594452	1.923332	-0.316557
C	3.803180	1.856681	0.399730
C	2.132057	3.172678	-0.765756
C	4.537915	3.017757	0.649496
H	4.180355	0.895065	0.753530
C	2.869657	4.331980	-0.508798
H	1.195724	3.255515	-1.322199
C	4.073058	4.257426	0.198148
H	5.480604	2.952159	1.198189
H	2.501830	5.296476	-0.867162
H	4.649688	5.164288	0.395557
C	2.767584	-0.942832	-0.906283
C	3.849258	-0.756201	-1.784467
C	2.540664	-2.214086	-0.353182

C	4.685728	-1.828332	-2.102465
H	4.044623	0.229233	-2.214331
C	3.378097	-3.285910	-0.675941
H	1.709483	-2.372536	0.339184
C	4.451084	-3.093059	-1.550628
H	5.526028	-1.675921	-2.784122
H	3.194723	-4.270180	-0.238440
H	5.108804	-3.928804	-1.801488
C	1.748542	0.071035	2.455119
C	0.746922	-0.491219	3.327157
C	0.795064	-1.983170	3.678483
C	-0.588115	-2.612879	3.899198
C	-1.508425	-2.503149	2.672749
C	-1.843911	-1.054330	2.284151
H	2.573458	-0.574036	2.130687
H	2.040046	1.118423	2.597491
H	0.423808	0.144428	4.167784
H	-0.539999	-0.490182	2.794174
H	1.315158	-2.525523	2.867874
H	1.419847	-2.112361	4.578750
H	-1.078467	-2.125208	4.761941
H	-0.462194	-3.672292	4.175270
H	-1.036084	-3.021649	1.815984
H	-2.445154	-3.055543	2.867894
H	-2.543661	-1.029911	1.440016
H	-2.354716	-0.544963	3.120750

^{4}TS5-6A-02
Geometry with 71 atoms:
Total energy: -2967.020052440

Cr	0.000772	-0.243280	1.260675
P	1.622972	0.266547	-0.543559
P	-1.484115	0.279320	-0.691680
C	-0.530828	1.057116	-2.093023
C	0.815070	0.340349	-2.226218
H	-1.118916	0.999509	-3.021536
H	-0.387294	2.123494	-1.856000
H	0.674732	-0.692492	-2.582177
H	1.480534	0.848319	-2.940683
C	3.099610	-0.789807	-0.758919
C	2.939190	-2.069850	-1.321253
C	4.360462	-0.406061	-0.272776
C	4.027742	-2.939633	-1.414101
H	1.963080	-2.400866	-1.686815
C	5.445517	-1.282617	-0.365929
H	4.501878	0.578091	0.178409
C	5.283417	-2.547408	-0.938039
H	3.893960	-3.929016	-1.858402
H	6.422833	-0.972592	0.011951
H	6.133784	-3.229748	-1.010042
C	2.195214	1.994212	-0.323749
C	3.081539	2.600562	-1.231361
C	1.669825	2.753121	0.734531
C	3.434535	3.942448	-1.074644
H	3.503802	2.023660	-2.058182
C	2.017600	4.098635	0.885662
H	0.984355	2.280906	1.445731
C	2.902027	4.692644	-0.019123
H	4.128158	4.406299	-1.780124
H	1.601544	4.680047	1.711805
H	3.179666	5.743023	0.097848
C	-2.027362	-1.312642	-1.420914
C	-1.541782	-2.508115	-0.865067
C	-2.847498	-1.368336	-2.561663
C	-1.867047	-3.741542	-1.436615
H	-0.904902	-2.472560	0.024932
C	-3.177105	-2.601663	-3.127625
H	-3.235616	-0.448081	-3.005724
C	-2.686861	-3.787753	-2.567633
H	-1.484311	-4.664595	-0.994886
H	-3.819259	-2.638376	-4.010955
H	-2.946746	-4.750226	-3.015019
C	-2.962723	1.326222	-0.450048
C	-4.258552	0.789164	-0.372619
C	-2.772974	2.702610	-0.221989
C	-5.347180	1.620540	-0.091090
H	-4.425477	-0.277200	-0.536149
C	-3.864499	3.527795	0.053487
H	-1.770352	3.138502	-0.256075
C	-5.154178	2.988446	0.118431
H	-6.351593	1.193740	-0.036883
H	-3.707306	4.596182	0.220822
H	-6.007609	3.635182	0.335958
C	1.792967	-0.458991	2.367458
C	0.724478	-0.635177	3.320427
C	0.432271	-2.019168	3.912540
C	-1.042452	-2.221696	4.286308
C	-1.981208	-2.143514	3.072022
C	-1.962297	-0.791571	2.337419
H	2.355996	-1.347056	2.053514
H	2.406346	0.447045	2.421407
H	0.598106	0.180173	4.051219
H	-0.551674	-0.488620	2.785697
H	0.733520	-2.792049	3.182090
H	1.076485	-2.163911	4.796361
H	-1.339639	-1.459102	5.029978
H	-1.162524	-3.198275	4.782488
H	-1.709251	-2.948353	2.363447
H	-3.013840	-2.369201	3.393526
H	-2.613160	-0.841898	1.455311
H	-2.372205	0.010852	2.976226

^{4}TS5-6A-03
Geometry with 71 atoms:
Total energy: -2967.016755480

Cr	0.063341	-0.583236	1.126242
P	1.637383	0.246241	-0.595458
P	-1.580055	0.228556	-0.643874
C	-0.641946	1.002921	-2.066084
C	0.752987	0.394166	-2.236721
H	-1.231108	0.922607	-2.992486
H	-0.569262	2.075105	-1.828943
H	0.697099	-0.634217	-2.629528
H	1.354477	0.986031	-2.943724
C	3.061329	-0.837860	-0.982220
C	3.817751	-0.664859	-2.156959
C	3.377920	-1.897582	-0.114953
C	4.874865	-1.530099	-2.446815
H	3.589751	0.148848	-2.849359
C	4.436211	-2.761914	-0.409103
H	2.796883	-2.051453	0.796324
C	5.186650	-2.577959	-1.573379
H	5.457624	-1.385756	-3.359780
H	4.672713	-3.581439	0.273681
H	6.014463	-3.253063	-1.803527
C	2.279798	1.936837	-0.273881
C	3.629040	2.289615	-0.432319
C	1.364676	2.910312	0.171823
C	4.048389	3.598619	-0.172051
H	4.362005	1.547754	-0.753440
C	1.786491	4.217498	0.420939
H	0.314567	2.653900	0.335973
C	3.130664	4.564909	0.247623
H	5.101736	3.861073	-0.297603
H	1.064021	4.963705	0.760455
H	3.462674	5.586577	0.447374
C	-2.686754	-1.027656	-1.389931
C	-3.871050	-1.379919	-0.716723
C	-2.326930	-1.727132	-2.554864
C	-4.684660	-2.401917	-1.209949
H	-4.166625	-0.847991	0.190801
C	-3.144443	-2.751289	-3.042427
H	-1.411485	-1.480511	-3.097171
C	-4.323265	-3.090698	-2.372386
H	-5.606322	-2.660345	-0.682812
H	-2.857974	-3.284153	-3.952426
H	-4.960795	-3.890790	-2.756054
C	-2.689348	1.567320	-0.068277
C	-3.685027	2.097313	-0.908085
C	-2.509229	2.105974	1.215721
C	-4.480439	3.156020	-0.467026
H	-3.843886	1.675937	-1.904037
C	-3.307136	3.167860	1.654037
H	-1.745860	1.693514	1.882288
C	-4.291156	3.693205	0.812377
H	-5.253281	3.563710	-1.123185
H	-3.162337	3.580559	2.655281
H	-4.916668	4.521492	1.154025
C	1.562065	0.009258	2.488128
C	0.604184	-0.727728	3.275593
C	0.953221	-2.108317	3.839068
C	-0.246169	-3.066790	3.888480
C	-0.828884	-3.356533	2.495983
C	-1.421057	-2.125657	1.785211
H	2.562028	-0.415486	2.342126
H	1.567870	1.103860	2.557355
H	-0.021082	-0.129611	3.958568
H	-0.515720	-1.185275	2.537749
H	1.751269	-2.558529	3.221637
H	1.381119	-1.978377	4.847655
H	-1.033811	-2.637611	4.535482
H	0.061960	-4.011820	4.363865
H	-0.031069	-3.793802	1.866385
H	-1.605506	-4.138006	2.575004
H	-1.686421	-2.375368	0.747068
H	-2.345625	-1.782863	2.280188

^{4}TS5-6A-04
Geometry with 71 atoms:
Total energy: -2967.013842570

Cr	0.057981	-0.443729	1.185666
P	1.631646	0.220885	-0.604255
P	-1.580484	0.175552	-0.652103
C	-0.655761	0.880228	-2.117888
C	0.751327	0.290726	-2.253320
H	-1.243156	0.731913	-3.037134
H	-0.603934	1.965561	-1.941179
H	0.718368	-0.751378	-2.610323
H	1.348029	0.866892	-2.977040
C	3.055381	-0.878018	-0.945343
C	3.815802	-0.743430	-2.122905
C	3.364081	-1.913460	-0.046906
C	4.869541	-1.621393	-2.384664
H	3.592697	0.049542	-2.840555
C	4.418568	-2.791477	-0.313732
H	2.780073	-2.039245	0.866575
C	5.173247	-2.645314	-1.480568
H	5.455361	-1.506120	-3.299818
H	4.648205	-3.592879	0.392486
H	5.997761	-3.331414	-1.689075
C	2.269342	1.926782	-0.356018
C	3.617739	2.279240	-0.519409
C	1.349522	2.909773	0.059005
C	4.032866	3.595478	-0.289581
H	4.354007	1.531016	-0.817463
C	1.766789	4.223620	0.277654
H	0.299697	2.652950	0.227373
C	3.111429	4.569361	0.103269
H	5.086293	3.857208	-0.416009
H	1.041398	4.976270	0.596036
H	3.440796	5.595748	0.282140
C	-2.651732	-1.152943	-1.316593
C	-3.893652	-1.419151	-0.712956
C	-2.204943	-1.982310	-2.360247
C	-4.677052	-2.487488	-1.155967
H	-4.260400	-0.782443	0.095425
C	-2.993229	-3.049508	-2.799439
H	-1.242756	-1.803011	-2.844672
C	-4.229710	-3.304631	-2.198814
H	-5.644339	-2.678910	-0.684993
H	-2.639368	-3.681728	-3.617418
H	-4.845347	-4.138268	-2.544996
C	-2.717110	1.526724	-0.162221
C	-3.696555	2.013949	-1.046132
C	-2.573832	2.120047	1.102788
C	-4.512989	3.080743	-0.666916
H	-3.827831	1.552590	-2.028202
C	-3.392946	3.189297	1.479446
H	-1.822516	1.745978	1.805092
C	-4.361562	3.669805	0.594498
H	-5.272756	3.454480	-1.357617
H	-3.275574	3.642918	2.466497
H	-5.003657	4.503899	0.887873
C	1.602836	0.122153	2.482200
C	0.608124	-0.491423	3.334583
C	0.890446	-1.838528	4.035114
C	0.268525	-3.077014	3.360290
C	-1.222274	-2.891088	3.039417
C	-1.442549	-1.916868	1.868211
H	2.571301	-0.378231	2.364698
H	1.685606	1.215687	2.483733
H	0.037612	0.215494	3.956050
H	-0.541024	-0.944031	2.640035

H	1.980134	-1.976578	4.126577
H	0.495708	-1.775554	5.061992
H	0.413523	-3.946929	4.020320
H	0.812160	-3.315049	2.424618
H	-1.683674	-3.864243	2.798683
H	-1.740185	-2.523655	3.944214
H	-1.232112	-2.441086	0.915823
H	-2.477109	-1.547742	1.818500

^{4}TS5-6A-05
Geometry with 71 atoms:
Total energy: -2967.012037800

Cr	-0.016485	0.038238	1.259970
P	-1.585412	0.350899	-0.666276
P	1.603172	0.365929	-0.595868
C	0.742147	0.526019	-2.254408
C	-0.677717	1.085910	-2.123713
H	1.352406	1.135197	-2.938921
H	0.714658	-0.492769	-2.669425
H	-0.667216	2.171321	-1.934569
H	-1.250304	0.921126	-3.049226
C	-3.026611	1.459639	-0.455614
C	-3.780511	1.897845	-1.560931
C	-3.367053	1.913265	0.830128
C	-4.858313	2.766261	-1.376755
H	-3.534413	1.558910	-2.570101
C	-4.447748	2.781800	1.009841
H	-2.788755	1.588048	1.698069
C	-5.194709	3.207147	-0.091793
H	-5.438841	3.099964	-2.240296
H	-4.704102	3.127246	2.014203
H	-6.039175	3.886204	0.048947
C	-2.219401	-1.270016	-1.256726
C	-3.583492	-1.524079	-1.470566
C	-1.290613	-2.312107	-1.448659
C	-4.005786	-2.789685	-1.891012
H	-4.324330	-0.739530	-1.307927
C	-1.716718	-3.570592	-1.876803
H	-0.225586	-2.154197	-1.258260
C	-3.076635	-3.811790	-2.100397
H	-5.070316	-2.974989	-2.054223
H	-0.983965	-4.367103	-2.027738
H	-3.411246	-4.798293	-2.430258
C	2.672409	1.847956	-0.441856
C	3.903169	1.755810	0.232633
C	2.233675	3.103611	-0.897010
C	4.682071	2.897213	0.436244
H	4.261280	0.789361	0.593344
C	3.016068	4.242924	-0.687570
H	1.280916	3.209698	-1.420336
C	4.240788	4.142929	-0.021200
H	5.640245	2.810828	0.954449
H	2.665798	5.212396	-1.050204
H	4.851356	5.034511	0.140313
C	2.741641	-1.045477	-0.855587
C	3.763641	-0.982088	-1.819708
C	2.546553	-2.234754	-0.135140
C	4.571329	-2.095611	-2.057715
H	3.933900	-0.058855	-2.379555
C	3.355065	-3.349513	-0.378252
H	1.765181	-2.292227	0.627274
C	4.366702	-3.280190	-1.339867
H	5.365278	-2.039547	-2.806492
H	3.196198	-4.270361	0.187909
H	5.000868	-4.149536	-1.529746
C	1.710945	0.294690	2.454167
C	0.675205	-0.133499	3.364818
C	0.690146	-1.574083	3.886184
C	-0.677468	-2.103179	4.382000
C	-1.910499	-1.481797	3.685645
C	-1.709619	-1.135337	2.198877
H	2.527252	-0.403850	2.234011
H	2.028328	1.343521	2.478425
H	0.330817	0.612160	4.099075
H	-0.567396	-0.286126	2.769115
H	1.060523	-2.217862	3.068981
H	1.440891	-1.658390	4.689082
H	-0.770594	-1.935256	5.467080
H	-0.688855	-3.197107	4.245877
H	-2.769212	-2.165038	3.798184
H	-2.200498	-0.557950	4.217941
H	-1.415007	-2.030411	1.618053
H	-2.648827	-0.756544	1.774290

^{4}TS5-6A-06
Geometry with 71 atoms:
Total energy: -2967.013820960

Cr	0.070180	-0.623681	1.145028
P	-1.407297	0.305993	-0.641231
P	1.695813	0.199517	-0.510751
C	0.938645	0.290893	-2.210083
C	-0.453450	0.924439	-2.130724
H	1.596835	0.841059	-2.899835
H	0.897560	-0.745740	-2.580579
H	-0.367352	2.013584	-1.992495
H	-1.032803	0.749859	-3.049910
C	-2.546771	1.676733	-0.240094
C	-3.390088	2.225092	-1.224066
C	-2.547213	2.223068	1.053249
C	-4.222189	3.301416	-0.912099
H	-3.402737	1.807397	-2.234158
C	-3.381851	3.301635	1.361040
H	-1.898429	1.803125	1.826080
C	-4.218910	3.840145	0.380207
H	-4.876643	3.721846	-1.679533
H	-3.377953	3.720374	2.370176
H	-4.871730	4.682599	0.621530
C	-2.441537	-1.081637	-1.254659
C	-3.816016	-1.161435	-0.976484
C	-1.810027	-2.163312	-1.897929
C	-4.543869	-2.297706	-1.344063
H	-4.325779	-0.338538	-0.472044
C	-2.542651	-3.292600	-2.268398
H	-0.738656	-2.136433	-2.111045
C	-3.911866	-3.363855	-1.989338
H	-5.612874	-2.346738	-1.123011
H	-2.041087	-4.122514	-2.772145
H	-4.483753	-4.250235	-2.274022
C	2.010035	1.948756	-0.060938
C	1.750142	2.353789	1.259575
C	2.465522	2.898573	-0.992012
C	1.940685	3.682714	1.646206
H	1.393757	1.619480	1.989132
C	2.655939	4.226748	-0.603564
H	2.676953	2.608678	-2.023819
C	2.393829	4.620164	0.713727
H	1.734767	3.985585	2.675576
H	3.011313	4.958655	-1.332937
H	2.542452	5.660724	1.012327
C	3.313505	-0.605413	-0.794708
C	4.539967	0.054847	-0.625806
C	3.304569	-1.963356	-1.162993
C	5.739524	-0.633159	-0.837816
H	4.565658	1.105161	-0.328798
C	4.503822	-2.642972	-1.381064
H	2.356564	-2.498332	-1.276121
C	5.724446	-1.977501	-1.218130
H	6.690754	-0.112185	-0.704208
H	4.487126	-3.696108	-1.672008
H	6.663907	-2.510350	-1.383834
C	1.799463	-1.336009	2.109425
C	0.730826	-1.567179	3.051065
C	0.191231	-2.995790	3.273529
C	-0.654230	-3.490897	2.087879
C	-2.004218	-2.752857	1.936059
C	-1.917336	-1.226628	2.150647
H	2.213772	-2.192398	1.562111
H	2.555833	-0.580424	2.349574
H	0.765100	-0.947710	3.960025
H	-0.519759	-1.081789	2.633187
H	1.042586	-3.674644	3.445616
H	-0.422139	-3.020071	4.189748
H	-0.836694	-4.573324	2.178699
H	-0.060241	-3.371935	1.158989
H	-2.410858	-2.964497	0.934240
H	-2.723119	-3.181476	2.656868
H	-2.661192	-0.680268	1.559137
H	-2.142782	-0.966972	3.200721

^{4}TS5-6B-01
Geometry with 79 atoms:
Total energy: -3195.929274260

Cr	-0.008213	-0.333025	1.165170
P	-1.510528	0.407374	-0.722646
P	1.580232	0.012145	-0.718196
O	0.020774	2.323158	0.969091
O	0.087533	-2.483506	-0.302304
C	0.775516	0.748142	-2.234349
C	-0.642782	0.189203	-2.357099
H	0.740894	1.841287	-2.111891
H	1.382407	0.528067	-3.125796
H	-1.210533	0.683990	-3.160055
H	-0.611575	-0.889680	-2.574973
C	-1.732075	2.229925	-0.630000
C	-2.679400	2.890959	-1.428026
C	-0.909715	2.996966	0.229423
C	-2.827255	4.277751	-1.378598
H	-3.320822	2.305024	-2.091042
C	-1.059883	4.390964	0.283661
C	-2.015403	5.020210	-0.518148
H	-3.572125	4.772904	-2.004885
H	-0.438187	4.993084	0.944940
H	-2.121813	6.106439	-0.464341
C	-3.189758	-0.274531	-0.972612
C	-3.404995	-1.368895	-1.829275
C	-4.263988	0.213179	-0.205150
C	-4.672467	-1.951035	-1.926372
H	-2.590192	-1.775065	-2.431900
C	-5.528151	-0.370872	-0.307382
H	-4.113748	1.058679	0.470050
C	-5.735932	-1.454069	-1.167623
H	-4.828760	-2.794429	-2.603540
H	-6.355091	0.022745	0.288660
H	-6.726282	-1.908656	-1.247887
C	2.070574	-1.658245	-1.307129
C	3.225229	-1.882826	-2.071724
C	1.229664	-2.755516	-1.006896
C	3.563790	-3.164972	-2.509555
H	3.875223	-1.040958	-2.320421
C	1.571180	-4.044852	-1.435926
C	2.736775	-4.241148	-2.181951
H	4.468931	-3.321000	-3.100010
H	0.938518	-4.898336	-1.194943
H	2.993647	-5.251199	-2.510380
C	3.128694	0.961411	-0.484514
C	3.169861	2.340464	-0.758035
C	4.254209	0.353294	0.102894
C	4.315411	3.087266	-0.466599
H	2.311609	2.850997	-1.198686
C	5.396430	1.103155	0.390900
H	4.242329	-0.713212	0.335378
C	5.431399	2.472161	0.107004
H	4.333427	4.156369	-0.692641
H	6.263352	0.613288	0.840959
H	6.326435	3.057053	0.332280
C	0.863621	3.039004	1.868285
H	1.524481	2.295914	2.329583
H	1.482763	3.778384	1.335630
H	0.273418	3.539590	2.653626
C	-0.881355	-3.509863	-0.098413
H	-1.748387	-3.026455	0.365741
H	-1.190819	-3.959220	-1.055796
H	-0.497000	-4.296274	0.571710
C	1.801874	-0.593593	2.234945
C	0.762094	-0.590831	3.238102
C	0.452721	-1.854086	4.049307
C	-1.016561	-1.944452	4.481730
C	-1.968405	-2.053319	3.280703
C	-1.932116	-0.856791	2.311450
H	2.289181	-1.551231	2.008150
H	2.483892	0.260219	2.187948
H	0.698752	0.326913	3.845598
H	-0.513961	-0.526759	2.718855
H	0.707819	-2.739988	3.440154
H	1.118682	-1.878562	4.928607
H	-1.278016	-1.054722	5.084713
H	-1.154099	-2.816123	5.141983
H	-1.713011	-2.973296	2.723856
H	-3.001962	-2.199328	3.642977
H	-2.527828	-1.096590	1.423183
H	-2.389270	0.037780	2.770675

^{4}TS5-6B-02

Geometry with 79 atoms:
Total energy: -3195.929479560

Cr	-0.027093	0.044851	1.210422
P	1.429084	-0.309350	-0.800854
P	-1.656865	-0.000442	-0.636083
O	0.103007	-2.508936	0.672524
O	-0.191425	2.508018	-0.068566
C	-0.910698	-0.642674	-2.223395
C	0.484742	-0.034558	-2.385447
H	-0.840901	-1.738914	-2.150377
H	-1.565276	-0.401784	-3.074819
H	1.030538	-0.479613	-3.231379
H	0.413536	1.049590	-2.562466
C	1.839771	-2.096944	-0.891269
C	2.839585	-2.585917	-1.746515
C	1.105606	-3.016713	-0.105459
C	3.132885	-3.949027	-1.811849
H	3.405907	-1.883812	-2.363189
C	1.404987	-4.385238	-0.161133
C	2.415795	-4.841129	-1.011357
H	3.917263	-4.310369	-2.479945
H	0.854842	-5.100876	0.448530
H	2.638466	-5.910418	-1.046027
C	3.008106	0.597614	-0.995702
C	3.016271	1.860277	-1.617676
C	4.198060	0.120121	-0.414624
C	4.188179	2.619517	-1.665210
H	2.108852	2.264559	-2.070284
C	5.365704	0.886018	-0.460678
H	4.222342	-0.859902	0.066012
C	5.365092	2.136603	-1.085372
H	4.180181	3.593577	-2.160692
H	6.281738	0.498905	-0.007938
H	6.280525	2.731930	-1.123294
C	-2.166517	1.699248	-1.104078
C	-3.330694	1.944510	-1.848418
C	-1.343195	2.793123	-0.744571
C	-3.698004	3.241482	-2.211710
H	-3.966663	1.105275	-2.139531
C	-1.716496	4.097756	-1.099517
C	-2.889276	4.313027	-1.828071
H	-4.610097	3.412344	-2.787157
H	-1.098723	4.949559	-0.817837
H	-3.166361	5.334783	-2.098948
C	-3.192832	-0.966933	-0.392404
C	-3.219032	-2.338098	-0.704986
C	-4.310253	-0.392444	0.241354
C	-4.344087	-3.111500	-0.404488
H	-2.362634	-2.817881	-1.182727
C	-5.432297	-1.169472	0.538218
H	-4.307930	0.667804	0.501858
C	-5.453284	-2.530353	0.216413
H	-4.352349	-4.174072	-0.659961
H	-6.294703	-0.707023	1.024561
H	-6.332664	-3.135762	0.449063
C	-0.612470	-3.361593	1.562366
H	0.062410	-3.812060	2.308872
H	-1.347881	-2.726159	2.072357
H	-1.149217	-4.154588	1.017382
C	0.669757	3.567477	0.333866
H	1.527596	3.096899	0.827817
H	1.033386	4.143238	-0.532688
H	0.166332	4.246492	1.041638
C	-1.720843	0.733779	2.280584
C	-0.667774	0.583087	3.259345
C	0.074995	1.805969	3.810411
C	1.508402	1.485807	4.266402
C	2.420889	0.969927	3.137699
C	1.895249	-0.298589	2.448624
H	-1.999104	1.748452	1.969848
H	-2.567742	0.041885	2.332812
H	-0.834198	-0.196734	4.020369
H	0.463172	-0.032718	2.781506
H	0.103174	2.589246	3.031967
H	-0.504008	2.228955	4.649566
H	1.466589	0.727480	5.070236
H	1.956282	2.385929	4.718390
H	2.548037	1.768744	2.383792
H	3.431310	0.789955	3.547813
H	2.566574	-0.619388	1.644555
H	1.857751	-1.140688	3.164490

^{4}TS5-6B-03
Geometry with 79 atoms:
Total energy: -3195.929164240

Cr	0.003936	0.229882	1.172277
P	1.491983	-0.363062	-0.772887
P	-1.594935	0.021923	-0.716334
O	0.003525	-2.390792	0.819387
O	-0.112970	2.494270	-0.084661
C	-0.812431	-0.669048	-2.264511
C	0.605045	-0.109413	-2.392716
H	-0.777277	-1.765004	-2.168095
H	-1.431888	-0.426874	-3.141522
H	1.163272	-0.589877	-3.210792
H	0.576576	0.973249	-2.594211
C	1.772364	-2.179816	-0.751824
C	2.746878	-2.779887	-1.565124
C	0.967679	-3.005073	0.069916
C	2.942682	-4.161668	-1.561980
H	3.370706	-2.149527	-2.203573
C	1.166811	-4.393571	0.078751
C	2.151333	-4.960986	-0.734125
H	3.708420	-4.609164	-2.198856
H	0.561296	-5.039393	0.713182
H	2.296287	-6.043924	-0.715747
C	3.141101	0.396200	-1.004030
C	3.284262	1.567600	-1.769703
C	4.257144	-0.102425	-0.306520
C	4.521502	2.213138	-1.850024
H	2.434073	1.986445	-2.312199
C	5.491392	0.545664	-0.391625
H	4.165384	-1.005584	0.300507
C	5.627558	1.703826	-1.163499
H	4.620659	3.116915	-2.456354
H	6.351052	0.142671	0.149370
H	6.594397	2.208447	-1.230047
C	-2.046590	1.726804	-1.227672
C	-3.163539	1.995586	-2.033668
C	-1.218915	2.802822	-0.830485
C	-3.477943	3.299017	-2.422510
H	-3.803096	1.169520	-2.353252
C	-1.536805	4.113685	-1.211696
C	-2.663683	4.352977	-2.002796
H	-4.353606	3.489121	-3.046458
H	-0.914613	4.951186	-0.898688
H	-2.900835	5.379502	-2.292715
C	-3.167572	-0.896092	-0.524761
C	-3.231401	-2.267623	-0.829287
C	-4.288369	-0.276950	0.059229
C	-4.396299	-2.996702	-0.572207
H	-2.375396	-2.783756	-1.268018
C	-5.450276	-1.009188	0.312321
H	-4.256942	0.783749	0.316195
C	-5.508515	-2.370579	-0.002894
H	-4.433098	-4.060032	-0.821970
H	-6.314252	-0.511770	0.759759
H	-6.418977	-2.941369	0.195046
C	-0.833651	-3.168641	1.671788
H	-1.542259	-2.470023	2.132323
H	-1.401561	-3.919392	1.099547
H	-0.245835	-3.666080	2.460919
C	0.832954	3.513908	0.231618
H	1.680263	3.010510	0.710234
H	1.188527	4.023650	-0.678178
H	0.404853	4.253717	0.927833
C	-1.791639	0.405557	2.280132
C	-0.743688	0.288958	3.268214
C	-0.409987	1.456130	4.203391
C	1.063795	1.477644	4.630463
C	2.011098	1.702424	3.441591
C	1.946319	0.623456	2.343274
H	-2.270158	1.386265	2.157377
H	-2.484965	-0.430750	2.153102
H	-0.684687	-0.687513	3.776130
H	0.527472	0.269458	2.731657
H	-0.657053	2.405215	3.694344
H	-1.068446	1.397309	5.086717
H	1.314598	0.524097	5.131944
H	1.218996	2.270399	5.380284
H	1.771036	2.684855	2.995509
H	3.049140	1.787062	3.810366
H	2.534536	0.955044	1.479551
H	2.397089	-0.322639	2.692464

^{4}TS5-6B-04
Geometry with 79 atoms:
Total energy: -3195.927361330

Cr	-0.082863	-0.318600	1.233144
P	-1.414335	0.382606	-0.767872
P	1.674314	-0.036873	-0.526488
O	-0.210339	2.198888	1.296983
O	0.290454	-2.565652	-0.777598
C	0.965507	0.578522	-2.151228
C	-0.472935	0.098987	-2.346173
H	0.998362	1.678663	-2.098034
H	1.606513	0.262390	-2.987542
H	-0.963972	0.620101	-3.182603
H	-0.495706	-0.980521	-2.548904
C	-1.529309	2.213947	-0.684895
C	-2.218464	2.934578	-1.674022
C	-0.889328	2.925540	0.356428
C	-2.286308	4.327206	-1.641425
H	-2.721497	2.388975	-2.476609
C	-0.956963	4.326548	0.392044
C	-1.652105	5.015698	-0.603990
H	-2.829545	4.869944	-2.417684
H	-0.464843	4.888650	1.184693
H	-1.694105	6.106895	-0.563726
C	-3.118650	-0.200828	-1.108228
C	-3.326098	-1.382036	-1.845560
C	-4.231965	0.455463	-0.551799
C	-4.615324	-1.892046	-2.019218
H	-2.486237	-1.915464	-2.295249
C	-5.518487	-0.061779	-0.724316
H	-4.100461	1.384080	0.007193
C	-5.714239	-1.236779	-1.455677
H	-4.760607	-2.805831	-2.600791
H	-6.372527	0.461646	-0.287619
H	-6.721429	-1.638118	-1.591088
C	2.452318	-1.645155	-0.964688
C	3.827082	-1.807020	-1.176603
C	1.614092	-2.783287	-1.030628
C	4.366986	-3.064274	-1.467621
H	4.490924	-0.943543	-1.105163
C	2.149919	-4.042521	-1.323746
C	3.525658	-4.174094	-1.543733
H	5.441564	-3.171475	-1.629715
H	1.509521	-4.922562	-1.379820
H	3.936594	-5.160625	-1.771618
C	3.051748	1.136186	-0.226391
C	3.826629	1.651698	-1.282295
C	3.313714	1.568681	1.083702
C	4.846753	2.570999	-1.025999
H	3.641042	1.336175	-2.311197
C	4.335145	2.488372	1.337769
H	2.713685	1.186712	1.909917
C	5.104079	2.989659	0.283824
H	5.443496	2.962037	-1.853702
H	4.529196	2.814272	2.362685
H	5.902990	3.708576	0.481481
C	0.267962	2.844714	2.474943
H	1.078941	3.552919	2.242613
H	-0.549288	3.365721	2.999994
H	0.660501	2.052719	3.125931
C	-0.607198	-3.663102	-0.693645
H	-0.731570	-4.158406	-1.671925
H	-0.271302	-4.405180	0.049583
H	-1.571496	-3.247120	-0.375627
C	1.456608	-1.401143	2.223182
C	0.307159	-1.450585	3.097780
C	-0.552707	-2.720124	3.173891
C	-2.019970	-2.447665	3.542666
C	-2.758367	-1.552944	2.529406
C	-2.099277	-0.179906	2.347376
H	1.711579	-2.303804	1.657429
H	2.338369	-0.842062	2.554773
H	0.421799	-0.948768	4.072822
H	-0.719487	-0.628442	2.723546
H	-0.512085	-3.233911	2.196994
H	-0.099995	-3.413501	3.903698
H	-2.057168	-1.968373	4.538513
H	-2.552486	-3.407351	3.644554

H	-2.806986	-2.072374	1.554195
H	-3.808544	-1.433315	2.852475
H	-2.648444	0.450544	1.639370
H	-2.099189	0.375195	3.304222

^{4}TS5-6B-05
Geometry with 79 atoms:
Total energy: -3195.926713080

Cr	0.020294	-0.170181	1.155558
P	-1.588582	0.347307	-0.742711
P	1.611215	0.056906	-0.732744
O	-0.455319	2.643954	0.433852
O	0.578197	-2.529578	-0.247279
C	0.685373	0.017885	-2.352899
C	-0.611977	0.824750	-2.260518
H	1.330670	0.352214	-3.179835
H	0.469910	-1.048153	-2.521846
H	-0.403650	1.897408	-2.135613
H	-1.234500	0.720151	-3.162034
C	-2.529375	1.873715	-0.360740
C	-3.887378	2.083164	-0.628897
C	-1.780508	2.910832	0.247166
C	-4.505242	3.288847	-0.280947
H	-4.470993	1.299928	-1.116020
C	-2.395898	4.116920	0.598953
C	-3.758895	4.294861	0.334781
H	-5.565421	3.439371	-0.495053
H	-1.826795	4.916763	1.072562
H	-4.235722	5.238076	0.612458
C	-2.790883	-0.923092	-1.281842
C	-2.561786	-1.701842	-2.430540
C	-3.890896	-1.237006	-0.459276
C	-3.415716	-2.761085	-2.751701
H	-1.716092	-1.495692	-3.088590
C	-4.745144	-2.292109	-0.787969
H	-4.086791	-0.652079	0.441322
C	-4.508613	-3.059376	-1.933101
H	-3.225265	-3.352981	-3.650368
H	-5.599049	-2.515907	-0.143917
H	-5.175899	-3.886262	-2.187723
C	2.612490	-1.475767	-0.799519
C	3.977142	-1.539675	-1.104053
C	1.910363	-2.674384	-0.528326
C	4.643738	-2.769051	-1.133378
H	4.526252	-0.621773	-1.323304
C	2.571890	-3.906088	-0.563041
C	3.938876	-3.942821	-0.862644
H	5.708608	-2.806445	-1.372371
H	2.039179	-4.834153	-0.356301
H	4.452335	-4.907102	-0.884314
C	2.765382	1.474437	-0.829735
C	3.805923	1.587755	0.112406
C	2.564470	2.521569	-1.745381
C	4.625364	2.718289	0.131358
H	3.985634	0.785532	0.829493
C	3.381140	3.656134	-1.716812
H	1.768962	2.469530	-2.489790
C	4.411657	3.759092	-0.778884
H	5.434461	2.786047	0.862771
H	3.210883	4.460884	-2.436226
H	5.050554	4.645325	-0.759914
C	0.410215	3.646061	0.954175
H	1.421829	3.225021	0.922898
H	0.384842	4.555544	0.331657
H	0.148322	3.901744	1.994679
C	-0.259977	-3.679802	-0.184973
H	0.003827	-4.326790	0.667338
H	-1.284668	-3.311532	-0.056779
H	-0.202590	-4.259206	-1.121172
C	1.667777	0.368982	2.362276
C	0.603406	0.064015	3.287829
C	0.699210	-1.167269	4.195484
C	-0.656444	-1.830279	4.476123
C	-1.318629	-2.358992	3.194893
C	-1.671029	-1.270209	2.166493
H	2.517182	-0.324665	2.316930
H	1.947692	1.416657	2.216070
H	0.139714	0.931472	3.784998
H	-0.586621	-0.366438	2.669605
H	1.369970	-1.906306	3.721678
H	1.184123	-0.869122	5.140733
H	-1.329834	-1.104153	4.968607
H	-0.518532	-2.657802	5.190768
H	-0.632942	-3.088092	2.725814
H	-2.230244	-2.926346	3.455154
H	-1.982550	-1.737343	1.224413
H	-2.512538	-0.647967	2.516495

^{4}TS5-6B-06
Geometry with 79 atoms:
Total energy: -3195.925347090

Cr	-0.099970	-0.706696	1.054072
P	-1.576040	0.253063	-0.712510
P	1.502505	0.234901	-0.616095
O	-0.960508	1.560896	1.871257
O	0.791383	-2.404600	-1.394436
C	0.694440	0.656937	-2.267066
C	-0.743611	0.142232	-2.370807
H	0.703464	1.755679	-2.320955
H	1.315847	0.278935	-3.092316
H	-1.315508	0.697168	-3.129923
H	-0.760649	-0.920214	-2.648924
C	-1.621791	2.052612	-0.353957
C	-1.961161	2.992171	-1.339643
C	-1.289553	2.511375	0.940834
C	-1.965555	4.359637	-1.062178
H	-2.233810	2.646592	-2.340203
C	-1.293249	3.883897	1.224001
C	-1.628460	4.797074	0.221125
H	-2.231110	5.077570	-1.840690
H	-1.032092	4.251428	2.215727
H	-1.624143	5.864988	0.452424
C	-3.314117	-0.234269	-1.017192
C	-4.381986	0.494582	-0.467504
C	-3.586737	-1.419277	-1.725839
C	-5.697159	0.052856	-0.636749
H	-4.190160	1.415087	0.088441
C	-4.903150	-1.853679	-1.896303
H	-2.772482	-2.010471	-2.153307
C	-5.961305	-1.118981	-1.351668
H	-6.519830	0.631277	-0.209111
H	-5.103098	-2.770918	-2.455718
H	-6.990705	-1.460641	-1.483957
C	2.702532	-1.103496	-0.992080
C	4.090844	-0.989274	-0.850628
C	2.154659	-2.358051	-1.346030
C	4.927227	-2.085422	-1.091264
H	4.529836	-0.038643	-0.544349
C	2.986229	-3.454683	-1.595538
C	4.372764	-3.308149	-1.469393
H	6.008341	-1.978578	-0.980902
H	2.568223	-4.420423	-1.878873
H	5.018778	-4.167560	-1.664424
C	2.490186	1.744715	-0.293412
C	3.387427	2.245680	-1.255998
C	2.274030	2.475393	0.884069
C	4.067981	3.443108	-1.028444
H	3.558352	1.699968	-2.187372
C	2.953588	3.676554	1.107817
H	1.559149	2.109715	1.619437
C	3.854007	4.159289	0.155178
H	4.766508	3.821073	-1.779003
H	2.775077	4.237594	2.028421
H	4.387268	5.096924	0.330422
C	-0.805149	1.936828	3.238590
H	-0.669434	1.005749	3.802319
H	0.079344	2.578776	3.384534
H	-1.703941	2.454039	3.610638
C	0.136055	-3.617709	-1.733715
H	0.375598	-3.927667	-2.765153
H	0.398461	-4.430388	-1.036325
H	-0.940946	-3.420570	-1.655739
C	1.628926	-0.744568	2.283248
C	0.649206	-1.552816	2.970565
C	0.811073	-3.075393	3.021179
C	-0.527520	-3.820639	3.108089
C	-1.421133	-3.584448	1.880243
C	-1.819325	-2.116361	1.651961
H	2.491957	-1.252832	1.837536
H	1.873653	0.236584	2.703398
H	0.255162	-1.137168	3.912388
H	-0.593813	-1.579799	2.364237
H	1.356928	-3.406679	2.119068
H	1.451590	-3.334478	3.881628
H	-1.065622	-3.500925	4.019996
H	-0.338703	-4.900286	3.225268
H	-0.890399	-3.958019	0.985414
H	-2.332399	-4.203862	1.968518
H	-2.392664	-2.019604	0.723037
H	-2.478005	-1.754896	2.462225

^{4}TS5-6B-07
Geometry with 79 atoms:
Total energy: -3195.925735870

Cr	0.022448	0.162231	1.187091
P	1.485485	-0.346093	-0.792215
P	-1.600263	0.024183	-0.688656
O	0.024014	-2.418173	0.755809
O	-0.159135	2.528179	-0.022481
C	-0.832789	-0.643793	-2.255184
C	0.578845	-0.071947	-2.396140
H	-0.787144	-1.740463	-2.171482
H	-1.465911	-0.397176	-3.121024
H	1.128580	-0.535489	-3.229572
H	0.541227	1.014103	-2.578627
C	1.798125	-2.156811	-0.802070
C	2.788669	-2.729042	-1.615850
C	1.004809	-3.006517	0.006063
C	3.011301	-4.106916	-1.624990
H	3.403446	-2.080112	-2.244369
C	1.231033	-4.390443	0.003230
C	2.231525	-4.929951	-0.809480
H	3.789151	-4.533061	-2.261819
H	0.634798	-5.053763	0.628487
H	2.398104	-6.009899	-0.800811
C	3.114133	0.458919	-1.003546
C	3.218026	1.662353	-1.724797
C	4.247744	-0.030390	-0.328721
C	4.432867	2.351117	-1.781141
H	2.353473	2.071991	-2.250871
C	5.459433	0.661679	-0.388681
H	4.190079	-0.961315	0.238678
C	5.556025	1.853181	-1.114159
H	4.500999	3.279815	-2.353168
H	6.333113	0.266013	0.135001
H	6.505423	2.392049	-1.160607
C	-2.073432	1.727971	-1.180207
C	-3.192464	1.980378	-1.989154
C	-1.266333	2.816049	-0.773196
C	-3.529940	3.278738	-2.374205
H	-3.815967	1.144142	-2.314063
C	-1.607908	4.122433	-1.153189
C	-2.735545	4.344915	-1.947608
H	-4.406879	3.455220	-3.000332
H	-1.003057	4.971098	-0.836766
H	-2.988973	5.368316	-2.234890
C	-3.166916	-0.904862	-0.494734
C	-3.232591	-2.269837	-0.826803
C	-4.281903	-0.299308	0.114220
C	-4.393369	-3.005964	-0.570896
H	-2.381098	-2.775145	-1.286409
C	-5.439683	-1.038460	0.366142
H	-4.248777	0.756433	0.391237
C	-5.499580	-2.393363	0.024191
H	-4.431847	-4.063956	-0.842158
H	-6.299156	-0.551663	0.833495
H	-6.406859	-2.969539	0.221149
C	-0.809820	-3.219226	1.589997
H	-0.224003	-3.708646	2.385599
H	-1.541348	-2.538342	2.041685
H	-1.351307	-3.978562	1.003976
C	0.741895	3.578838	0.318638
H	1.123961	4.085013	-0.582764
H	0.264011	4.317385	0.982753
H	1.581500	3.112537	0.845649
C	-1.729236	0.398431	2.324372
C	-0.682439	0.160343	3.297710
C	-0.299838	1.247946	4.330215
C	0.979979	2.040294	4.009887
C	2.157949	1.118878	3.660180
C	1.989789	0.482404	2.266514
H	-2.138564	1.415777	2.256462
H	-2.482846	-0.380731	2.176860

H -0.696998 -0.853152 3.726519
H 0.590643 0.086261 2.741537
H -1.147030 1.942223 4.451449
H -0.159348 0.752609 5.304896
H 1.227835 2.677423 4.874132
H 0.794578 2.727502 3.163081
H 3.107001 1.681128 3.699304
H 2.238285 0.334605 4.435482
H 2.300768 1.215011 1.506638
H 2.623848 -0.408819 2.142279

^{4}TS5-6B-08
Geometry with 79 atoms:
Total energy: -3195.925646660
Cr -0.139201 -0.725334 1.031360
P -1.543862 0.367040 -0.720427
P 1.525297 0.166905 -0.609328
O -0.815974 1.596898 1.874054
O 0.576588 -2.444004 -1.202062
C 0.749782 0.684614 -2.247770
C -0.702383 0.218431 -2.372641
H 0.792004 1.784011 -2.259499
H 1.362576 0.318176 -3.084582
H -1.246620 0.786465 -3.142674
H -0.751496 -0.845542 -2.644155
C -1.466276 2.160169 -0.338743
C -1.749301 3.135697 -1.307421
C -1.085665 2.577436 0.956836
C -1.651653 4.496104 -1.013070
H -2.055697 2.825385 -2.309532
C -0.986741 3.943004 1.256978
C -1.267465 4.891427 0.270752
H -1.874547 5.241381 -1.779166
H -0.686230 4.274567 2.250308
H -1.183476 5.953140 0.515177
C -3.306175 0.003264 -1.052024
C -3.645665 -1.151634 -1.780928
C -4.330862 0.796509 -0.509869
C -4.985228 -1.493939 -1.978514
H -2.864816 -1.789216 -2.203583
C -5.669833 0.447070 -0.706685
H -4.085041 1.695702 0.059728
C -6.000191 -0.695418 -1.441471
H -5.237190 -2.388338 -2.553700
H -6.459049 1.074715 -0.285441
H -7.048018 -0.964159 -1.595697
C 2.600802 -1.261044 -1.037837
C 4.000178 -1.235995 -1.043585
C 1.940257 -2.483028 -1.301610
C 4.735250 -2.388931 -1.342714
H 4.527982 -0.310932 -0.807779
C 2.668726 -3.635621 -1.610879
C 4.067525 -3.578247 -1.633742
H 5.826623 -2.351927 -1.346877
H 2.163689 -4.577186 -1.825693
H 4.633449 -4.481481 -1.874346
C 2.633413 1.581211 -0.258037
C 3.517048 2.071536 -1.238296
C 2.534560 2.252878 0.969825
C 4.302717 3.196176 -0.979337
H 3.592383 1.575708 -2.209492
C 3.319788 3.380990 1.225142
H 1.830013 1.900581 1.722351
C 4.207825 3.850613 0.254333
H 4.989544 3.566190 -1.744502
H 3.233120 3.896443 2.184803
H 4.822751 4.731479 0.454610
C -0.646685 1.948939 3.245668
H -0.573809 1.006049 3.801116
H 0.274322 2.533771 3.404277
H -1.514648 2.517006 3.617211
C -0.191278 -3.586436 -1.555447
H 0.044146 -4.449663 -0.911550
H -1.243528 -3.311555 -1.407724
H -0.029761 -3.862763 -2.611149
C 1.597223 -0.977005 2.223985
C 0.539000 -1.650094 2.939874
C 0.520530 -3.178961 3.038361
C -0.896922 -3.751156 3.173057
C -1.764930 -3.468556 1.937018
C -1.976933 -1.976943 1.623197
H 2.370236 -1.595758 1.752629
H 1.986618 -0.042521 2.640271
H 0.207808 -1.165963 3.872812
H -0.700209 -1.575673 2.327414
H 1.002706 -3.600875 2.138019
H 1.143729 -3.484609 3.896139
H -1.380392 -3.322262 4.070749
H -0.840731 -4.838657 3.343494
H -1.290737 -3.954810 1.065952
H -2.746724 -3.961186 2.058716
H -2.502220 -1.870548 0.667032
H -2.617007 -1.497825 2.385649

^{4}TS5-6B-09
Geometry with 79 atoms:
Total energy: -3195.925642750
Cr -0.057273 -0.414013 1.129155
P 1.554049 0.013927 -0.718518
P -1.514373 0.416844 -0.718647
O 0.162399 -2.544791 -0.488699
O -0.045250 2.187581 1.198051
C -0.678956 0.181386 -2.368106
C 0.751111 0.714123 -2.258541
H -0.677749 -0.897194 -2.588336
H -1.244952 0.691425 -3.162668
H 1.355389 0.459080 -3.142093
H 0.731338 1.810518 -2.171536
C 2.180799 -1.609290 -1.304346
C 3.402811 -1.760022 -1.975879
C 1.369286 -2.749932 -1.101090
C 3.836122 -3.014218 -2.412343
H 4.028941 -0.883658 -2.155847
C 1.804245 -4.010332 -1.531354
C 3.036275 -4.134440 -2.180329
H 4.792656 -3.113384 -2.929555
H 1.193189 -4.897246 -1.368282
H 3.366053 -5.122604 -2.510300
C 3.011885 1.076628 -0.402969
C 2.945671 2.461481 -0.639887
C 4.158221 0.550430 0.222473
C 4.007953 3.294891 -0.277535
H 2.064488 2.908294 -1.103838
C 5.217132 1.387015 0.582217
H 4.226788 -0.518889 0.430743
C 5.146450 2.761240 0.332812
H 3.943255 4.367543 -0.476673
H 6.101858 0.960676 1.061341
H 5.976825 3.413738 0.613245
C -1.616717 2.245116 -0.585875
C -2.426985 2.985802 -1.461611
C -0.835470 2.935494 0.371479
C -2.477276 4.378614 -1.400128
H -3.036765 2.457787 -2.199279
C -0.885512 4.336832 0.434734
C -1.703025 5.046376 -0.448199
H -3.115835 4.936614 -2.087946
H -0.293627 4.882315 1.168543
H -1.731748 6.136920 -0.384879
C -3.230835 -0.172900 -0.942533
C -3.484451 -1.333259 -1.696501
C -4.293879 0.440814 -0.256737
C -4.778353 -1.855178 -1.777355
H -2.676336 -1.839575 -2.228472
C -5.585344 -0.085255 -0.340420
H -4.117397 1.340065 0.337435
C -5.831572 -1.232559 -1.100825
H -4.963861 -2.751165 -2.374945
H -6.403700 0.406061 0.191559
H -6.843103 -1.640380 -1.166776
C -0.773213 -3.615779 -0.404189
H -0.978550 -4.042656 -1.399733
H -0.416829 -4.411403 0.270224
H -1.698896 -3.187785 -0.001783
C 0.768303 2.836221 2.173902
H 1.327106 2.044828 2.687500
H 1.486493 3.524605 1.701824
H 0.150384 3.379639 2.907458
C 1.717116 -0.815323 2.181615
C 0.668154 -0.858330 3.181249
C 0.330349 -2.173723 3.923345
C -0.993138 -2.845851 3.510446
C -2.150708 -1.841142 3.401202
C -2.011519 -0.964666 2.141168
H 2.186407 -1.765358 1.891741
H 2.421847 0.021624 2.214145
H 0.645639 0.022608 3.841108
H -0.599354 -0.680353 2.668016
H 1.162390 -2.884909 3.795670
H 0.278649 -1.944820 5.000324
H -1.229919 -3.638519 4.238166
H -0.868343 -3.350589 2.534330
H -3.117533 -2.373137 3.379725
H -2.169543 -1.214130 4.312005
H -2.325641 -1.561971 1.271200
H -2.657371 -0.073778 2.180226

^{4}TS5-6B-10
Geometry with 79 atoms:
Total energy: -3195.927437870
Cr -0.060255 -0.408188 1.163099
P 1.451232 -0.100445 -0.840991
P -1.657599 0.019633 -0.671202
O 0.230712 -2.663412 -0.323159
O -0.402735 2.249250 0.915165
C -0.911846 -0.421277 -2.320685
C 0.485107 0.192374 -2.416600
H -0.853089 -1.518321 -2.364985
H -1.562094 -0.079046 -3.140899
H 1.036383 -0.202879 -3.282809
H 0.419014 1.286658 -2.531182
C 2.263278 -1.735754 -1.085181
C 3.590459 -1.897216 -1.503646
C 1.511662 -2.887686 -0.752621
C 4.160743 -3.169642 -1.612391
H 4.194301 -1.018623 -1.737744
C 2.077439 -4.162322 -0.857751
C 3.400964 -4.294918 -1.292548
H 5.196615 -3.276051 -1.941094
H 1.502428 -5.052204 -0.602390
H 3.836975 -5.293586 -1.373297
C 2.771926 1.165095 -0.923906
C 3.131242 1.850956 0.248017
C 3.396887 1.510796 -2.136822
C 4.104250 2.853706 0.213365
H 2.645805 1.603334 1.191570
C 4.368252 2.514273 -2.168564
H 3.130089 0.998471 -3.063924
C 4.724561 3.186092 -0.994173
H 4.376040 3.377733 1.133087
H 4.848386 2.773422 -3.115370
H 5.484488 3.970955 -1.022178
C -1.966541 1.822649 -0.822873
C -2.868504 2.306312 -1.784654
C -1.284128 2.748250 0.000374
C -3.103215 3.672307 -1.938208
H -3.406440 1.593332 -2.414656
C -1.523219 4.123855 -0.149380
C -2.426243 4.574916 -1.114249
H -3.810280 4.028474 -2.690084
H -1.008530 4.850152 0.478224
H -2.599774 5.648869 -1.218106
C -3.323386 -0.747257 -0.697973
C -4.388562 -0.139269 -0.009299
C -3.533456 -1.995081 -1.311433
C -5.636840 -0.761869 0.054980
H -4.245435 0.829531 0.474243
C -4.785051 -2.615013 -1.243604
H -2.726954 -2.496336 -1.850161
C -5.838993 -2.001163 -0.561392
H -6.456409 -0.274566 0.588821
H -4.936097 -3.581092 -1.731795
H -6.816850 -2.486095 -0.511576
C -0.569565 -3.741689 0.148497
H -0.087424 -4.256895 0.996335
H -1.514352 -3.294716 0.484210
H -0.779739 -4.467480 -0.654510
C 0.239966 3.137914 1.822636
H 0.866668 2.517460 2.473966
H 0.882762 3.859594 1.293360
H -0.495851 3.676491 2.442418
C -1.835794 -0.423001 2.319788
C -0.792488 -0.866447 3.213254

C -0.275832 0.037892 4.337486
C 1.177102 -0.268977 4.731920
C 2.181873 -0.042995 3.587998
C 1.907397 -0.882842 2.329731
H -2.224580 0.595953 2.443016
H -2.594270 -1.148255 2.008308
H -0.848398 -1.926198 3.511059
H 0.438973 -0.993502 2.620553
H -0.357916 1.091776 4.015844
H -0.939181 -0.068787 5.212918
H 1.244203 -1.319464 5.070841
H 1.461006 0.350803 5.598090
H 2.171940 1.031063 3.323360
H 3.202941 -0.244672 3.959126
H 2.641768 -0.662002 1.546274
H 2.024002 -1.959111 2.553028

^{4}TS5-6B-11
Geometry with 79 atoms:
Total energy: -3195.926574560
Cr 0.084394 -0.280674 1.094958
P -1.535760 0.145370 -0.787513
P 1.616956 0.435416 -0.700087
O -1.336440 1.975953 1.543782
O 1.290866 -2.351378 -0.657047
C 0.787779 0.245550 -2.365086
C -0.629235 0.821807 -2.277264
H 1.378090 0.747712 -3.146655
H 0.777088 -0.830368 -2.589232
H -0.591152 1.913125 -2.129547
H -1.210813 0.639096 -3.194190
C -2.712962 1.469868 -0.328628
C -3.845698 1.743653 -1.111181
C -2.460612 2.261268 0.816495
C -4.724857 2.773250 -0.773535
H -4.045147 1.129707 -1.992831
C -3.347374 3.292647 1.159738
C -4.469116 3.541248 0.364406
H -5.602237 2.972069 -1.392295
H -3.174698 3.907842 2.041744
H -5.149641 4.348656 0.645500
C -2.570141 -1.231777 -1.415055
C -3.758561 -1.581885 -0.748072
C -2.123124 -2.036584 -2.478096
C -4.488887 -2.703795 -1.147091
H -4.121944 -0.971742 0.081650
C -2.856923 -3.159359 -2.872401
H -1.200177 -1.797349 -3.009314
C -4.040372 -3.496043 -2.208613
H -5.414106 -2.958916 -0.624583
H -2.501849 -3.771076 -3.705474
H -4.613199 -4.373168 -2.519156
C 3.009534 -0.751824 -0.725794
C 4.367699 -0.419369 -0.667172
C 2.636452 -2.117197 -0.679211
C 5.345077 -1.419302 -0.607504
H 4.670768 0.628737 -0.656958
C 3.609460 -3.119853 -0.630767
C 4.962540 -2.761043 -0.599389
H 6.401405 -1.145694 -0.566146
H 3.326799 -4.172138 -0.605875
H 5.720688 -3.546939 -0.558460
C 2.283101 2.137660 -0.774108
C 3.193619 2.539899 -1.769446
C 1.789786 3.093454 0.128867
C 3.618358 3.868115 -1.838761
H 3.572730 1.815950 -2.495029
C 2.211229 4.424191 0.051982
H 1.061883 2.794884 0.883554
C 3.129829 4.811437 -0.927046
H 4.330139 4.170262 -2.610808
H 1.819094 5.159914 0.758527
H 3.462845 5.850564 -0.985634
C -1.046626 2.752551 2.702869
H -0.936281 3.820219 2.452111
H -1.827443 2.630305 3.471831
H -0.093896 2.382585 3.098038
C 0.793620 -3.682980 -0.682753
H -0.300746 -3.602431 -0.677200
H 1.112881 -4.208628 -1.598385
H 1.122206 -4.253979 0.201183
C 1.719717 0.232334 2.339481
C 0.763274 -0.417335 3.205956
C 1.072444 -1.793130 3.805520
C -0.185482 -2.641651 4.034655
C -0.907195 -2.979391 2.721163
C -1.423827 -1.761378 1.932499
H 2.645988 -0.306859 2.106182
H 1.865461 1.314160 2.428907
H 0.230933 0.238137 3.913585
H -0.391634 -0.851790 2.561654
H 1.758570 -2.333269 3.128602
H 1.620010 -1.648865 4.752440
H -0.875467 -2.101327 4.709729
H 0.088318 -3.573616 4.555457
H -0.208130 -3.547828 2.081613
H -1.748640 -3.664761 2.928823
H -1.763049 -2.089835 0.942723
H -2.289621 -1.295790 2.435111

^{4}TS5-6B-12
Geometry with 79 atoms:
Total energy: -3195.922380410
Cr -0.138180 -0.715394 1.019227
P -1.502464 0.375780 -0.770432
P 1.563128 0.121775 -0.604549
O -0.777418 1.743517 1.765111
O 0.607132 -2.508317 -1.112721
C 0.818377 0.673108 -2.245093
C -0.626320 0.190283 -2.399545
H 0.848031 1.773020 -2.238816
H 1.447718 0.325624 -3.077582
H -1.152447 0.736775 -3.196952
H -0.656028 -0.880827 -2.646527
C -1.468589 2.183043 -0.461809
C -1.794228 3.102213 -1.471756
C -1.076974 2.669990 0.805900
C -1.726465 4.477191 -1.246025
H -2.111897 2.733315 -2.450508
C -1.005188 4.051844 1.034929
C -1.327292 4.943433 0.009425
H -1.983570 5.178585 -2.042289
H -0.693957 4.440371 2.003755
H -1.264714 6.017502 0.200688
C -3.251310 -0.045416 -1.095142
C -4.289079 0.686794 -0.494284
C -3.567968 -1.184339 -1.857540
C -5.619133 0.293867 -0.665671
H -4.059650 1.571846 0.103875
C -4.899629 -1.570292 -2.029613
H -2.778541 -1.776216 -2.327677
C -5.927695 -0.832927 -1.433788
H -6.418494 0.874429 -0.198569
H -5.134898 -2.451162 -2.632141
H -6.968686 -1.136371 -1.568572
C 2.628399 -1.303542 -1.055654
C 4.024634 -1.262796 -1.134728
C 1.966541 -2.535090 -1.267743
C 4.756804 -2.413262 -1.450119
H 4.552647 -0.327753 -0.941036
C 2.692660 -3.685818 -1.589230
C 4.088024 -3.614623 -1.683071
H 5.846073 -2.365624 -1.510406
H 2.188919 -4.636558 -1.761555
H 4.650826 -4.516964 -1.934206
C 2.671410 1.515507 -0.179315
C 3.514243 2.102313 -1.141397
C 2.622970 2.063450 1.112680
C 4.306533 3.202569 -0.807008
H 3.552000 1.703157 -2.157861
C 3.415271 3.166457 1.443702
H 1.952740 1.633340 1.857806
C 4.260213 3.734531 0.486584
H 4.960817 3.648711 -1.559987
H 3.370227 3.583920 2.452681
H 4.880060 4.596471 0.745497
C -0.610130 2.164293 3.115991
H -1.489994 2.727372 3.467600
H -0.509640 1.250200 3.714302
H 0.296036 2.779336 3.241339
C -0.150650 -3.693259 -1.318422
H 0.159401 -4.496902 -0.630434
H -1.196786 -3.433995 -1.110372
H -0.063347 -4.047314 -2.359304
C 1.580230 -1.281262 2.091598
C 0.477504 -1.543331 2.993753
C 0.175026 -2.985912 3.466963
C -0.915314 -3.727799 2.676289
C -2.210818 -2.909304 2.577749
C -2.061552 -1.722359 1.609563
H 2.074599 -2.145587 1.629158
H 2.278781 -0.477065 2.341036
H 0.377721 -0.801557 3.799956
H -0.789153 -1.375249 2.395620
H 1.110211 -3.568778 3.453148
H -0.146756 -2.935703 4.520149
H -1.105244 -4.698315 3.162322
H -0.554082 -3.958551 1.656213
H -3.045455 -3.552591 2.248708
H -2.483561 -2.551956 3.587912
H -2.142036 -2.103758 0.577993
H -2.852253 -0.967973 1.740144

^{4}TS5-6C-01
Geometry with 83 atoms:
Total energy: -3124.185817810
Cr -0.006356 -0.038947 1.288896
P 1.637597 0.414958 -0.532893
P -1.461080 -0.042152 -0.751939
C -0.537210 0.609368 -2.235589
C 0.888921 0.060602 -2.205637
H -1.061009 0.348380 -3.166296
H -0.537648 1.707499 -2.171838
H 0.890898 -1.030717 -2.341381
H 1.507584 0.482669 -3.011270
C 3.228613 -0.508152 -0.499451
C 3.211828 -1.914614 -0.328529
C 4.457572 0.173509 -0.556064
C 4.440540 -2.587979 -0.239554
C 5.665389 -0.519645 -0.467281
C 5.656466 -1.907442 -0.309787
H 4.438063 -3.672846 -0.100987
H 6.609984 0.027322 -0.513906
H 6.596175 -2.459736 -0.232172
C 2.037490 2.206722 -0.635645
C 1.738128 3.046634 0.450434
C 2.601638 2.772791 -1.794170
C 1.991916 4.419511 0.381960
H 1.296698 2.633194 1.359180
C 2.855213 4.144283 -1.861257
H 2.858621 2.144417 -2.649415
C 2.549471 4.970729 -0.774402
H 1.751501 5.058230 1.235235
H 3.295782 4.569394 -2.766294
H 2.747777 6.043850 -0.829944
C -3.067094 0.856108 -0.727948
C -3.106861 2.234220 -0.400504
C -4.263950 0.165104 -0.995050
C -4.356808 2.874806 -0.391650
C -5.493594 0.823277 -0.964095
C -5.538823 2.187510 -0.668450
H -4.397830 3.942220 -0.156123
H -6.411645 0.270216 -1.176184
H -6.494474 2.717144 -0.651290
C -1.837105 -1.780066 -1.234119
C -2.172302 -2.131697 -2.554444
C -1.780445 -2.791598 -0.260040
C -2.440159 -3.461394 -2.887507
H -2.239419 -1.369949 -3.333581
C -2.054950 -4.120883 -0.592854
H -1.522490 -2.546405 0.770260
C -2.384089 -4.458781 -1.908106
H -2.698239 -3.718740 -3.917635
H -2.008469 -4.892737 0.179148
H -2.596072 -5.497893 -2.171348
C 1.775124 -0.034266 2.436911
C 0.702019 -0.093913 3.399163
C 0.450352 -1.371869 4.208751
C -1.017165 -1.544221 4.623019
C -1.964101 -1.693804 3.421154
C -1.971165 -0.490403 2.461473
H 2.351070 -0.948834 2.249625
H 2.386446 0.872252 2.378184

H	0.542327	0.823113	3.989315
H	-0.552747	-0.101301	2.839952
H	0.767411	-2.244388	3.608472
H	1.103130	-1.356158	5.097946
H	-1.328906	-0.673932	5.229911
H	-1.111760	-2.425438	5.277783
H	-1.683118	-2.610904	2.870208
H	-2.990714	-1.874203	3.787313
H	-2.643997	-0.679412	1.615386
H	-2.372709	0.401921	2.972999
H	4.478702	1.258750	-0.663344
H	-4.239726	-0.899689	-1.232008
C	1.936358	-2.729521	-0.238364
C	1.686827	-3.629627	-1.454194
H	1.067242	-2.063439	-0.097747
H	1.978507	-3.355382	0.669751
H	0.737598	-4.176113	-1.347109
H	1.640198	-3.046263	-2.387291
H	2.494975	-4.367929	-1.572735
C	-1.888258	3.053865	-0.017499
C	-1.814671	3.364028	1.483260
H	-1.908184	4.002533	-0.579615
H	-0.955288	2.558761	-0.320488
H	-2.712921	3.899789	1.826990
H	-1.739689	2.440683	2.079333
H	-0.939514	3.993562	1.708374

^{4}TS5-6C-02
Geometry with 83 atoms:
Total energy: -3124.185804030

Cr	0.013362	-0.057829	1.286653
P	1.599174	0.501808	-0.544271
P	-1.478679	-0.082391	-0.748130
C	-0.627638	0.790720	-2.153872
C	0.828661	0.332630	-2.238284
H	-1.170543	0.641317	-3.099081
H	-0.685437	1.865593	-1.924260
H	0.899109	-0.723717	-2.537324
H	1.396880	0.914584	-2.978602
C	3.205299	-0.385519	-0.645814
C	3.213735	-1.800468	-0.724793
C	4.420207	0.321508	-0.595752
C	4.456622	-2.449533	-0.799999
C	5.641604	-0.350431	-0.653861
C	5.658810	-1.742273	-0.768051
H	4.478347	-3.539449	-0.882578
H	6.575506	0.215126	-0.613808
H	6.608782	-2.279114	-0.826930
C	1.941204	2.306433	-0.454129
C	2.556246	3.008790	-1.507217
C	1.517648	3.019382	0.679598
C	2.743811	4.389750	-1.419128
H	2.901218	2.479875	-2.398773
C	1.704705	4.401617	0.767345
H	1.029720	2.484565	1.498373
C	2.319318	5.088288	-0.282851
H	3.225442	4.923892	-2.241706
H	1.367751	4.940688	1.655895
H	2.467921	6.168882	-0.218520
C	-3.167543	0.638340	-0.670274
C	-3.368924	1.906710	-0.073093
C	-4.269308	-0.092743	-1.152040
C	-4.681280	2.399579	0.008649
C	-5.562672	0.421413	-1.062089
C	-5.768811	1.673862	-0.477826
H	-4.848931	3.375971	0.472325
H	-6.406610	-0.158803	-1.442541
H	-6.778624	2.083244	-0.394802
C	-1.675258	-1.815367	-1.336871
C	-1.775218	-2.841567	-0.379302
C	-1.688031	-2.157271	-2.700527
C	-1.880748	-4.176848	-0.775217
H	-1.768878	-2.601682	0.684856
C	-1.783720	-3.495057	-3.093842
H	-1.625724	-1.385572	-3.469871
C	-1.878283	-4.507125	-2.133769
H	-1.959165	-4.961183	-0.018482
H	-1.787050	-3.746183	-4.157289
H	-1.951956	-5.552030	-2.444655
C	1.830734	-0.078503	2.381399
C	0.783981	-0.133329	3.374206
C	0.549285	-1.412688	4.188286
C	-0.909757	-1.593754	4.627878
C	-1.878412	-1.731315	3.441777
C	-1.912158	-0.509898	2.506038
H	2.395855	-0.995484	2.174765
H	2.450186	0.821788	2.315946
H	0.649871	0.782913	3.972068
H	-0.486549	-0.131663	2.852424
H	0.859309	-2.284229	3.583775
H	1.217221	-1.394812	5.066045
H	-1.213728	-0.732051	5.250820
H	-0.988688	-2.483205	5.273565
H	-1.595896	-2.633367	2.866236
H	-2.895904	-1.929727	3.823836
H	-2.604584	-0.682445	1.673906
H	-2.297343	0.376064	3.042449
H	4.418979	1.408613	-0.506645
H	-4.118246	-1.076907	-1.599033
C	1.954342	-2.648794	-0.712015
C	1.859680	-3.614203	0.476204
H	1.896528	-3.224649	-1.651914
H	1.056674	-2.014897	-0.708467
H	1.867079	-3.069661	1.433865
H	0.927077	-4.197067	0.421233
H	2.698830	-4.326188	0.496110
C	-2.241843	2.771844	0.454332
C	-1.936679	3.988171	-0.429493
H	-1.323856	2.171249	0.578467
H	-2.506673	3.120503	1.466915
H	-2.816652	4.644732	-0.512729
H	-1.107237	4.578883	-0.011715
H	-1.655752	3.688146	-1.451414

^{4}TS5-6C-03
Geometry with 83 atoms:
Total energy: -3124.186783080

Cr	-0.000121	-0.052039	1.330384
P	1.631759	0.411083	-0.495412
P	-1.458688	-0.108729	-0.711513
C	-0.557823	0.611648	-2.168714
C	0.883244	0.104330	-2.174731
H	-1.087493	0.387913	-3.106895
H	-0.590118	1.704040	-2.041532
H	0.918723	-0.980904	-2.350825
H	1.484699	0.573766	-2.967043
C	3.234726	-0.485511	-0.505311
C	3.239402	-1.894820	-0.362835
C	4.450548	0.217062	-0.578111
C	4.479221	-2.551092	-0.308942
C	5.669707	-0.459790	-0.525485
C	5.683113	-1.850192	-0.389867
H	4.495918	-3.638254	-0.191088
H	6.605734	0.100662	-0.583668
H	6.632196	-2.389541	-0.339767
C	2.000253	2.213346	-0.515280
C	1.795996	2.967313	0.653620
C	2.449880	2.871389	-1.674780
C	2.033763	4.344470	0.665662
H	1.448036	2.480224	1.567040
C	2.684629	4.248132	-1.662300
H	2.629181	2.312951	-2.595767
C	2.477050	4.987640	-0.493092
H	1.868803	4.914791	1.582822
H	3.033838	4.745553	-2.570389
H	2.660694	6.064729	-0.486798
C	-3.104154	0.708312	-0.725635
C	-3.239369	2.027181	-0.226954
C	-4.234734	0.013326	-1.193120
C	-4.518425	2.606544	-0.229980
C	-5.493823	0.613364	-1.187068
C	-5.634913	1.916809	-0.703445
H	-4.637127	3.622858	0.156254
H	-6.361951	0.061187	-1.554646
H	-6.617488	2.394786	-0.688292
C	-1.738750	-1.868617	-1.167357
C	-1.780752	-2.320258	-2.497662
C	-1.898770	-2.803096	-0.127713
C	-1.974557	-3.675901	-2.778114
H	-1.668118	-1.621367	-3.328388
C	-2.097961	-4.156217	-0.410222
H	-1.873406	-2.472457	0.912496
C	-2.134082	-4.595716	-1.737248
H	-2.001756	-4.014067	-3.816712
H	-2.223078	-4.868512	0.408816
H	-2.284914	-5.654677	-1.960361
C	1.786812	-0.232307	2.452902
C	0.732174	-0.107507	3.430668
C	0.311985	-1.302471	4.294887
C	-1.151293	-1.222101	4.752803
C	-2.149438	-1.272143	3.583621
C	-1.984449	-0.145024	2.548568
H	2.221681	-1.225605	2.283060
H	2.520516	0.574098	2.354492
H	0.713757	0.844438	3.985915
H	-0.515800	0.033906	2.889247
H	0.467956	-2.234080	3.720493
H	0.986871	-1.360205	5.165609
H	-1.301581	-0.287194	5.324089
H	-1.363359	-2.047069	5.451813
H	-2.043886	-2.252202	3.082014
H	-3.178921	-1.255078	3.984276
H	-2.692082	-0.282366	1.722482
H	-2.226767	0.833647	3.000847
H	4.449688	1.304302	-0.671934
H	-4.133159	-1.008663	-1.562883
C	1.973724	-2.724876	-0.272902
C	1.719599	-3.609330	-1.499099
H	1.100154	-2.069260	-0.115877
H	2.029579	-3.363663	0.625231
H	0.774815	-4.163421	-1.391088
H	1.660783	-3.012928	-2.423151
H	2.530917	-4.341153	-1.635865
C	-2.074873	2.851405	0.285843
C	-1.646242	3.976019	-0.665327
H	-1.209541	2.198422	0.495552
H	-2.354988	3.291211	1.257771
H	-0.790430	4.532606	-0.253338
H	-1.350461	3.584451	-1.651143
H	-2.469765	4.687827	-0.831895

^{4}TS5-6C-04
Geometry with 83 atoms:
Total energy: -3124.185469250

Cr	0.060095	-0.390147	1.198060
P	1.633986	0.312918	-0.613730
P	-1.568485	0.150392	-0.702711
C	-0.581050	0.103846	-2.283210
C	0.680958	0.945665	-2.092616
H	-0.314573	-0.942749	-2.498041
H	-1.186940	0.469540	-3.125731
H	1.320099	0.923749	-2.987428
H	0.414619	1.997600	-1.907100
C	2.719975	-0.982707	-1.361268
C	2.649019	-2.360291	-1.047812
C	3.651358	-0.536278	-2.324006
C	3.525688	-3.236029	-1.718081
C	4.505539	-1.422390	-2.973359
C	4.441436	-2.785201	-2.665005
H	3.480830	-4.302720	-1.481136
H	5.220781	-1.051073	-3.710870
H	5.108404	-3.495138	-3.160256
C	2.759102	1.686795	-0.149337
C	2.257889	2.998255	-0.065937
C	4.072453	1.430107	0.279457
C	3.062673	4.033685	0.416195
H	1.233513	3.226348	-0.369192
C	4.872485	2.468626	0.763381
H	4.478283	0.417445	0.233411
C	4.372063	3.772138	0.831218
H	2.662959	5.049460	0.467145
H	5.893893	2.255694	1.088175
H	5.000535	4.582698	1.207856
C	-2.282659	1.858597	-0.764584
C	-2.038736	2.855620	0.208736
C	-3.092922	2.157375	-1.878758
C	-2.610718	4.126846	0.011633
C	-3.650430	3.422046	-2.050416
C	-3.401831	4.415500	-1.098625
H	-2.427105	4.905177	0.757465
H	-4.275520	3.630579	-2.921760
H	-3.827916	5.414483	-1.219575
C	-3.016973	-0.936980	-0.972100

C	-4.156248	-0.745749	-0.168811
C	-2.991432	-2.009252	-1.879622
C	-5.248642	-1.607315	-0.276332
H	-4.196684	0.088126	0.537226
C	-4.089056	-2.870326	-1.982856
H	-2.123022	-2.183769	-2.517161
C	-5.217238	-2.672916	-1.182875
H	-6.129991	-1.444217	0.348634
H	-4.060671	-3.696946	-2.697033
H	-6.073120	-3.346963	-1.266148
C	1.659688	0.115434	2.475937
C	0.663136	-0.477745	3.331796
C	0.912047	-1.827585	4.012522
C	-0.360959	-2.671129	4.171531
C	-0.971585	-3.061631	2.816440
C	-1.444595	-1.874076	1.958120
H	2.588498	-0.439628	2.294678
H	1.802739	1.201105	2.499450
H	0.106937	0.225662	3.970916
H	-0.475158	-0.940787	2.644571
H	1.652948	-2.395933	3.422755
H	1.375659	-1.640438	4.995835
H	-1.104427	-2.109775	4.767664
H	-0.127860	-3.581549	4.746709
H	-0.216252	-3.638424	2.252659
H	-1.818625	-3.751925	2.976393
H	-1.679619	-2.217698	0.940932
H	-2.369306	-1.432060	2.365771
H	3.718271	0.528991	-2.557983
H	-3.300092	1.382535	-2.621268
C	1.659516	-2.986596	-0.086578
C	0.399736	-3.526201	-0.775088
H	1.378866	-2.274823	0.707768
H	2.160428	-3.814061	0.440956
H	-0.186529	-2.718310	-1.237207
H	0.662920	-4.241391	-1.569690
H	-0.255090	-4.042049	-0.056693
C	-1.268028	2.621613	1.491336
C	-2.140180	2.019742	2.600391
H	-0.851562	3.580099	1.838395
H	-0.385809	1.983161	1.304932
H	-2.538062	1.034123	2.310331
H	-1.570166	1.897984	3.534823
H	-3.000753	2.672798	2.813520

^{4}TS5-6C-05
Geometry with 83 atoms:
Total energy: -3124.186022830

Cr	0.060975	-0.043337	1.244925
P	1.629218	0.263278	-0.676837
P	-1.643065	0.081002	-0.672445
C	-0.736015	0.692116	-2.181932
C	0.685709	0.126521	-2.284569
H	-1.325633	0.473121	-3.086258
H	-0.725701	1.787058	-2.075767
H	0.664798	-0.949766	-2.513301
H	1.253239	0.609000	-3.095879
C	2.993998	-0.961768	-0.880185
C	2.987682	-2.224609	-0.238653
C	4.052586	-0.623639	-1.746308
C	4.061186	-3.097720	-0.489779
C	5.101603	-1.509868	-1.982945
C	5.106496	-2.753645	-1.346033
H	4.070795	-4.073541	0.003507
H	5.913379	-1.226941	-2.657088
H	5.926108	-3.456486	-1.514726
C	2.471446	1.896332	-0.751649
C	2.003546	2.946898	-1.558782
C	3.581310	2.126149	0.083473
C	2.624822	4.199990	-1.523463
H	1.154819	2.808468	-2.229362
C	4.201457	3.375687	0.111892
H	3.975603	1.319720	0.704438
C	3.721682	4.419089	-0.687501
H	2.248374	5.005517	-2.158642
H	5.066226	3.534238	0.760771
H	4.206595	5.397861	-0.662419
C	-3.079098	1.237246	-0.558569
C	-3.156128	2.279889	0.396984
C	-4.111802	1.079743	-1.504194
C	-4.279145	3.125715	0.361431
C	-5.211757	1.935280	-1.521249
C	-5.295739	2.963765	-0.579166
H	-4.351801	3.931850	1.096924
H	-6.001183	1.794745	-2.263340
H	-6.155045	3.638933	-0.574414
C	-2.414929	-1.509502	-1.172438
C	-3.413120	-2.054799	-0.342560
C	-2.013516	-2.226420	-2.311987
C	-3.987306	-3.290844	-0.643227
H	-3.759700	-1.502724	0.533934
C	-2.589485	-3.466125	-2.608073
H	-1.252053	-1.831310	-2.985767
C	-3.572855	-4.003203	-1.773900
H	-4.765642	-3.697440	0.007042
H	-2.268263	-4.010316	-3.499530
H	-4.022218	-4.971313	-2.007652
C	1.571196	0.903507	2.371043
C	0.590388	0.482518	3.340310
C	0.919061	-0.620575	4.352352
C	-0.283841	-1.507765	4.703552
C	-0.814824	-2.277115	3.484146
C	-1.353496	-1.386958	2.349072
H	2.542715	0.394725	2.372881
H	1.632093	1.963200	2.102185
H	-0.037311	1.281906	3.764794
H	-0.487948	-0.233125	2.780475
H	1.727056	-1.252478	3.942813
H	1.325588	-0.147774	5.262346
H	-1.091214	-0.884589	5.131182
H	0.005851	-2.220951	5.491810
H	0.000697	-2.910856	3.091290
H	-1.608883	-2.974876	3.803684
H	-1.513886	-1.995444	1.447792
H	-2.323803	-0.938296	2.619770
H	4.062619	0.352681	-2.235810
H	-4.061282	0.267571	-2.233013
C	1.859880	-2.720712	0.641632
C	0.707818	-3.342814	-0.154781
H	1.477629	-1.895698	1.272186
H	2.257576	-3.461480	1.352686
H	-0.089468	-3.710522	0.509681
H	0.257197	-2.613245	-0.842561
H	1.062931	-4.190251	-0.761328
C	-2.072410	2.574929	1.413124
C	-0.897643	3.370545	0.828593
H	-1.707709	1.634790	1.861415
H	-2.512271	3.143434	2.247183
H	-0.143799	3.595341	1.599079
H	-0.391965	2.818574	0.020828
H	-1.243358	4.325551	0.403223

^{4}TS5-6C-06
Geometry with 83 atoms:
Total energy: -3124.185545200

Cr	0.093748	-0.716412	1.016760
P	1.554240	0.428707	-0.638451
P	-1.602677	0.059796	-0.714570
C	-0.672508	0.090214	-2.331291
C	0.607401	0.916129	-2.187506
H	-0.441671	-0.956482	-2.581388
H	-1.309799	0.474613	-3.141038
H	1.263676	0.790198	-3.061106
H	0.364374	1.986174	-2.118102
C	2.999165	-0.518884	-1.285349
C	3.163444	-1.911865	-1.095077
C	3.958392	0.199974	-2.028683
C	4.309133	-2.523323	-1.637846
C	5.080563	-0.429857	-2.561114
C	5.259956	-1.801341	-2.356071
H	4.450653	-3.597422	-1.488574
H	5.814590	0.148508	-3.126933
H	6.140462	-2.308693	-2.757833
C	2.233231	2.004440	0.019795
C	1.403964	3.138434	0.087624
C	3.506017	2.055557	0.614705
C	1.847890	4.304531	0.716275
H	0.396878	3.123274	-0.333824
C	3.945492	3.224702	1.241444
H	4.161729	1.183069	0.591096
C	3.120469	4.352491	1.292853
H	1.191252	5.177322	0.754432
H	4.940294	3.251857	1.692800
H	3.467636	5.264963	1.783537
C	-2.225495	1.792174	-0.557941
C	-2.098013	2.557892	0.626177
C	-2.851290	2.356545	-1.687158
C	-2.589680	3.875796	0.618365
C	-3.331088	3.664816	-1.670744
C	-3.193064	4.430580	-0.509881
H	-2.494413	4.476870	1.526581
H	-3.811714	4.081639	-2.558807
H	-3.560382	5.459314	-0.481380
C	-3.090973	-0.954349	-1.051592
C	-4.357413	-0.565041	-0.583699
C	-2.952672	-2.194886	-1.702253
C	-5.464664	-1.396535	-0.775039
H	-4.486867	0.393798	-0.077283
C	-4.063669	-3.018871	-1.895686
H	-1.977209	-2.528501	-2.064548
C	-5.321979	-2.622102	-1.432018
H	-6.445431	-1.080174	-0.411557
H	-3.944005	-3.975593	-2.409943
H	-6.190281	-3.267787	-1.583383
C	1.659483	-0.267918	2.359124
C	0.740930	-1.093319	3.105630
C	1.133817	-2.502763	3.558792
C	-0.041583	-3.491140	3.561498
C	-0.620937	-3.713663	2.155221
C	-1.227508	-2.456256	1.505626
H	2.637520	-0.690930	2.097768
H	1.695193	0.806029	2.570171
H	0.125234	-0.562966	3.849628
H	-0.360386	-1.553557	2.348258
H	1.929081	-2.885108	2.895355
H	1.577458	-2.432310	4.566305
H	-0.835468	-3.119627	4.235951
H	0.291565	-4.454795	3.979141
H	0.184365	-4.104456	1.507596
H	-1.387947	-4.507221	2.192726
H	-1.425638	-2.643208	0.440097
H	-2.195317	-2.196238	1.965490
H	3.832364	1.274596	-2.180906
H	-2.979213	1.762383	-2.594861
C	2.148178	-2.806823	-0.416279
C	1.114744	-3.387964	-1.387301
H	1.635015	-2.260006	0.392784
H	2.675284	-3.631698	0.088311
H	1.604007	-3.986701	-2.170841
H	0.395729	-4.035749	-0.861840
H	0.552337	-2.587395	-1.891465
C	-1.506387	2.019335	1.911158
C	-2.468228	1.105635	2.681014
H	-1.216990	2.865909	2.552320
H	-0.554760	1.499630	1.695746
H	-3.385022	1.650985	2.954591
H	-2.772235	0.232764	2.081804
H	-2.006064	0.735013	3.609554

^{4}TS5-6C-07
Geometry with 83 atoms:
Total energy: -3124.183615680

Cr	0.027365	-0.202970	1.260825
P	1.638277	0.192069	-0.607765
P	-1.591559	0.158968	-0.683387
C	-0.591113	0.029023	-2.247738
C	0.696285	0.837791	-2.083143
H	-0.350370	-1.033959	-2.406745
H	-1.172260	0.368809	-3.117541
H	1.322409	0.791459	-2.986596
H	0.455914	1.897234	-1.902076
C	2.493913	-1.303196	-1.290911
C	2.321361	-2.621677	-0.809851
C	3.382844	-1.064967	-2.361223
C	3.050483	-3.653182	-1.434902
C	4.085665	-2.101846	-2.966528
C	3.917191	-3.408503	-2.496393
H	2.928217	-4.675863	-1.067366
H	4.768044	-1.890879	-3.793146
H	4.467172	-4.234761	-2.953503
C	3.018465	1.377647	-0.360998
C	2.924976	2.728657	-0.734049
C	4.179682	0.931011	0.296180

C	3.972284	3.613055	-0.454192
H	2.043140	3.111539	-1.249724
C	5.221633	1.816637	0.573609
H	4.277308	-0.118883	0.581955
C	5.120259	3.161470	0.200774
H	3.887731	4.659896	-0.755939
H	6.118733	1.453860	1.081198
H	5.937181	3.854032	0.417222
C	-2.368133	1.836348	-0.814415
C	-2.277771	2.840416	0.177229
C	-3.124973	2.077714	-1.981141
C	-2.936928	4.063346	-0.059374
C	-3.762771	3.295814	-2.193369
C	-3.663788	4.298709	-1.222861
H	-2.876935	4.844974	0.703243
H	-4.343227	3.458640	-3.104415
H	-4.164313	5.259107	-1.369036
C	-3.025041	-0.963021	-0.905550
C	-4.125767	-0.801356	-0.043353
C	-3.041709	-2.006869	-1.845576
C	-5.217636	-1.666401	-0.120043
H	-4.136180	0.012801	0.686012
C	-4.139029	-2.871649	-1.918472
H	-2.209929	-2.155805	-2.535828
C	-5.225795	-2.706206	-1.056648
H	-6.066685	-1.527390	0.553539
H	-4.142846	-3.676000	-2.658202
H	-6.080773	-3.384000	-1.115761
C	1.640083	0.407658	2.475306
C	0.577208	0.092543	3.396682
C	0.701127	-1.099358	4.352750
C	-0.631138	-1.814442	4.618073
C	-1.225883	-2.424925	3.339448
C	-1.598212	-1.398882	2.254663
H	2.508593	-0.261820	2.447880
H	1.896324	1.455167	2.291207
H	0.069728	0.957148	3.853370
H	-0.569132	-0.421805	2.773047
H	1.420799	-1.823005	3.930468
H	1.140883	-0.740530	5.298622
H	-1.352982	-1.102291	5.059592
H	-0.478462	-2.605679	5.369542
H	-0.494880	-3.143836	2.925299
H	-2.120006	-3.020931	3.594647
H	-1.845874	-1.916459	1.318119
H	-2.489032	-0.818327	2.546739
H	3.538322	-0.043275	-2.716282
H	-3.233530	1.288613	-2.729329
C	1.364678	-3.033413	0.290460
C	0.022698	-3.543127	-0.248459
H	1.201331	-2.205898	1.004581
H	1.837536	-3.828817	0.888522
H	-0.637494	-3.873796	0.567558
H	-0.506451	-2.762201	-0.814097
H	0.174184	-4.395317	-0.928967
C	-1.497029	2.722548	1.470801
C	-0.122057	3.398074	1.405324
H	-1.390385	1.665833	1.767699
H	-2.087170	3.187672	2.277118
H	0.529276	2.917289	0.660022
H	-0.219379	4.458152	1.124089
H	0.391565	3.352362	2.378083

^{4}TS5-6C-08
Geometry with 83 atoms:
Total energy: -3124.182956340

Cr	-0.271635	-1.293549	0.735566
P	1.512010	0.119182	-0.421809
P	-1.638817	0.080501	-0.836074
C	-0.535818	0.263982	-2.327300
C	0.779560	0.944064	-1.934618
H	-0.347292	-0.756871	-2.698751
H	-1.046893	0.810009	-3.134050
H	1.498782	0.899930	-2.763131
H	0.614568	2.007136	-1.706652
C	2.882610	-0.946262	-1.023334
C	4.007951	-0.488318	-1.753762
C	2.763072	-2.313957	-0.707757
C	4.970229	-1.440292	-2.133048
C	3.726055	-3.239930	-1.104503
C	4.839129	-2.794170	-1.821592
H	5.850427	-1.103068	-2.687406
H	3.612514	-4.295957	-0.849249
H	5.611300	-3.501044	-2.135133
C	2.257916	1.443421	0.603703
C	1.560815	2.644570	0.823612
C	3.462194	1.213904	1.291948
C	2.069337	3.604161	1.702262
H	0.613061	2.840904	0.319421
C	3.965457	2.177597	2.169855
H	4.014586	0.284353	1.138454
C	3.272551	3.374357	2.376862
H	1.518607	4.535005	1.858849
H	4.905875	1.990451	2.694037
H	3.669314	4.125917	3.063626
C	-1.994719	1.826224	-0.341861
C	-1.944047	2.271082	1.000670
C	-2.326339	2.736516	-1.364402
C	-2.218040	3.625603	1.261584
C	-2.589848	4.075814	-1.082627
C	-2.531795	4.522329	0.240782
H	-2.179775	3.979541	2.295264
H	-2.842303	4.765239	-1.891502
H	-2.734737	5.569499	0.478382
C	-3.228831	-0.537151	-1.504826
C	-4.454457	-0.041968	-1.028645
C	-3.230898	-1.578853	-2.449679
C	-5.658868	-0.577531	-1.494231
H	-4.474605	0.772010	-0.301243
C	-4.437231	-2.104134	-2.918138
H	-2.291438	-1.988078	-2.828577
C	-5.653823	-1.606474	-2.440087
H	-6.605813	-0.182070	-1.118795
H	-4.426155	-2.907575	-3.658811
H	-6.596596	-2.020371	-2.805692
C	-1.803465	-2.729658	0.542108
C	-0.919859	-3.262791	1.547157
C	-1.359449	-3.316406	3.014319
C	-0.217925	-3.076768	4.013355
C	0.421507	-1.687874	3.858803
C	1.114284	-1.463420	2.503472
H	-2.794358	-2.372371	0.846154
H	-1.795228	-3.174097	-0.460359
H	-0.308173	-4.128299	1.244966
H	0.212804	-2.441860	1.800024
H	-2.145447	-2.558407	3.176011
H	-1.831934	-4.295727	3.201627
H	0.557652	-3.854540	3.883121
H	-0.603309	-3.194717	5.038912
H	-0.360866	-0.920418	4.004610
H	1.152179	-1.525459	4.671169
H	1.461921	-0.423815	2.419975
H	2.005633	-2.106076	2.405214
H	1.898380	-2.648604	-0.127766
H	-2.390051	2.394410	-2.400050
C	4.239560	0.956045	-2.155191
C	4.202779	1.181677	-3.673115
H	5.226909	1.265206	-1.771475
H	3.516605	1.620859	-1.665082
H	4.974053	0.589347	-4.189626
H	3.229345	0.894607	-4.103385
H	4.379563	2.242367	-3.911734
C	-1.658867	1.358267	2.173798
C	-2.875805	0.527137	2.599078
H	-1.313148	1.965529	3.024168
H	-0.802127	0.701117	1.936463
H	-2.634064	-0.117587	3.458544
H	-3.708851	1.183733	2.894974
H	-3.239113	-0.114995	1.781258

^{4}TS5-6C-09
Geometry with 83 atoms:
Total energy: -3124.183027400

Cr	0.283665	-0.529024	1.262871
P	1.673958	0.387636	-0.594317
P	-1.503388	0.126400	-0.413859
C	-0.695290	0.319704	-2.081533
C	0.584030	1.143148	-1.914239
H	-0.457908	-0.688154	-2.457357
H	-1.378356	0.790964	-2.803180
H	1.141242	1.211716	-2.860091
H	0.341475	2.170000	-1.602823
C	2.681982	-0.826973	-1.557659
C	2.644249	-2.226084	-1.355058
C	3.509598	-0.293742	-2.569248
C	3.448871	-3.036515	-2.179809
C	4.292627	-1.116013	-3.373966
C	4.262064	-2.500215	-3.174602
H	3.430142	-4.119299	-2.027613
H	4.927830	-0.679102	-4.147953
H	4.875420	-3.160302	-3.792860
C	2.838102	1.726653	-0.125905
C	4.189377	1.448451	0.140979
C	2.343970	3.020150	0.121667
C	5.033619	2.451333	0.624985
H	4.590763	0.447824	-0.032245
C	3.193524	4.019884	0.602338
H	1.290372	3.258109	-0.045565
C	4.540237	3.739040	0.853790
H	6.083678	2.222808	0.823420
H	2.798757	5.022941	0.782030
H	5.203201	4.521908	1.229966
C	-2.049222	1.835035	0.011742
C	-3.018891	2.588824	-0.696033
C	-1.351979	2.432166	1.082115
C	-3.232177	3.920297	-0.296422
C	-1.581732	3.754125	1.459983
C	-2.529609	4.503194	0.758389
H	-3.971954	4.515960	-0.838507
H	-1.024205	4.192854	2.290573
H	-2.722839	5.543386	1.032174
C	-2.986872	-0.911987	-0.636249
C	-3.949864	-0.917727	0.388806
C	-3.147965	-1.771352	-1.735922
C	-5.061459	-1.757924	0.307282
H	-3.836889	-0.253306	1.249633
C	-4.262743	-2.612257	-1.811361
H	-2.416119	-1.787400	-2.545964
C	-5.220231	-2.607147	-0.793147
H	-5.807814	-1.748026	1.105342
H	-4.383233	-3.272308	-2.673759
H	-6.090537	-3.264651	-0.856333
C	1.909414	0.028853	2.479321
C	0.989991	-0.640208	3.365002
C	1.341292	-1.999647	3.977995
C	0.125958	-2.919986	4.162252
C	-0.537934	-3.285216	2.825184
C	-1.122012	-2.088761	2.053592
H	2.856060	-0.469687	2.235239
H	1.999399	1.119741	2.530798
H	0.433973	0.012037	4.057819
H	-0.167808	-1.130807	2.717129
H	2.081782	-2.502715	3.330834
H	1.842195	-1.826295	4.945489
H	-0.613387	-2.428424	4.821765
H	0.439137	-3.839653	4.682083
H	0.212560	-3.794466	2.193514
H	-1.336820	-4.027811	2.998947
H	-1.414697	-2.397980	1.040320
H	-2.033005	-1.705514	2.542543
H	3.551434	0.787832	-2.719803
H	-0.603056	1.850430	1.630054
C	1.753026	-2.932328	-0.354657
C	0.443154	-3.445087	-0.966118
H	1.542152	-2.273101	0.506553
H	2.306251	-3.783641	0.073342
H	0.646945	-4.120360	-1.811547
H	-0.151834	-3.999566	-0.224823
H	-0.178203	-2.619680	-1.345914
C	-3.861688	2.054271	-1.837398
C	-5.340017	1.880426	-1.461563
H	-3.476314	1.093436	-2.198293
H	-3.785258	2.758142	-2.683955
H	-5.915238	1.503615	-2.322000
H	-5.456934	1.162003	-0.636520
H	-5.791288	2.834266	-1.145924

^{4}TS5-6C-10
Geometry with 83 atoms:
Total energy: -3124.185168070

Cr	0.004871	-0.654612	1.132485
P	-1.591741	-0.228321	-0.757958
P	1.601404	0.092419	-0.716340

C 0.653626 0.286548 -2.322892
C -0.621345 -0.559652 -2.316667
H 0.402429 1.350721 -2.443375
H 1.308078 0.011298 -3.162515
H -1.236268 -0.361797 -3.206986
H -0.385069 -1.635110 -2.327745
C -2.157361 1.516755 -1.002719
C -2.040178 2.515045 -0.007093
C -2.709627 1.850030 -2.255803
C -2.463223 3.819971 -0.319228
C -3.123775 3.149083 -2.542795
C -2.992779 4.142246 -1.567818
H -2.372770 4.597759 0.443906
H -3.547485 3.383658 -3.521979
H -3.308083 5.167131 -1.778283
C -3.107552 -1.243750 -0.936532
C -2.983479 -2.612819 -1.235961
C -4.384200 -0.707993 -0.700409
C -4.117071 -3.424025 -1.314411
H -2.000145 -3.058243 -1.406188
C -5.515662 -1.526857 -0.771676
H -4.502233 0.352069 -0.467058
C -5.386096 -2.883210 -1.081285
H -4.008156 -4.484272 -1.555627
H -6.503807 -1.097800 -0.588281
H -6.272136 -3.519939 -1.139779
C 3.033794 -0.968461 -1.198909
C 3.246301 -2.280308 -0.713066
C 3.931419 -0.418280 -2.138233
C 4.365590 -2.987210 -1.192328
C 5.030551 -1.139219 -2.597186
C 5.248939 -2.434138 -2.117000
H 4.541915 -4.001031 -0.822602
H 5.714892 -0.691167 -3.321363
H 6.109465 -3.012392 -2.462383
C 2.319004 1.747791 -0.372290
C 3.597184 1.875329 0.199892
C 1.518651 2.895522 -0.516730
C 4.069461 3.129015 0.597894
H 4.230631 0.996376 0.335538
C 1.995830 4.146112 -0.116965
H 0.511762 2.826076 -0.933111
C 3.272566 4.266918 0.440399
H 5.067721 3.214645 1.034112
H 1.363146 5.028301 -0.242416
H 3.645476 5.245398 0.752500
C -1.446785 -2.017283 1.823864
C -0.455511 -1.968310 2.869024
C -0.770895 -1.324072 4.222104
C 0.446152 -0.647095 4.868961
C 0.997665 0.510766 4.021366
C 1.519347 0.098551 2.632753
H -2.431018 -1.572695 2.014708
H -1.493756 -2.901485 1.178360
H 0.189442 -2.857197 2.960297
H 0.606167 -1.104964 2.592395
H -1.573999 -0.579545 4.086293
H -1.178337 -2.100218 4.891955
H 1.242344 -1.397778 5.030148
H 0.168318 -0.272907 5.867438
H 0.199942 1.266519 3.898522
H 1.806797 1.019635 4.574869
H 1.759122 0.993794 2.044129
H 2.448291 -0.491416 2.716048
H -2.829142 1.080391 -3.021376
H 3.773410 0.598280 -2.507345
C -1.546208 2.244265 1.396188
C -2.642174 1.685717 2.311328
H -1.144666 3.175297 1.824368
H -0.683239 1.554303 1.364897
H -3.492257 2.383225 2.368065
H -3.026429 0.723524 1.938004
H -2.264272 1.530882 3.333554
C 2.312623 -3.001963 0.236294
C 1.157757 -3.713519 -0.480683
H 1.913167 -2.303336 0.987665
H 2.892125 -3.745346 0.805851
H 1.537392 -4.441869 -1.214093
H 0.516641 -4.252732 0.234492
H 0.527518 -2.995831 -1.029104

^{4}TS5-6C-11
Geometry with 83 atoms:
Total energy: -3124.184163600
Cr 0.006275 0.102385 1.244813
P 1.600144 0.260484 -0.678568
P -1.619739 0.050074 -0.720931
C -0.624277 -0.037929 -2.298385
C 0.623558 0.835846 -2.160072
H -0.341016 -1.088038 -2.468508
H -1.240976 0.273889 -3.153813
H 1.246809 0.799223 -3.066157
H 0.339318 1.887210 -1.998067
C 2.363872 -1.299771 -1.322627
C 2.133012 -2.582118 -0.773804
C 3.187951 -1.167789 -2.458942
C 2.733575 -3.690009 -1.401394
C 3.772903 -2.278296 -3.061722
C 3.539040 -3.550155 -2.529577
H 2.561716 -4.686212 -0.984325
H 4.407952 -2.151792 -3.941557
H 3.987243 -4.432596 -2.992723
C 3.019897 1.410030 -0.542531
C 2.942410 2.744506 -0.973134
C 4.186422 0.964982 0.105012
C 4.015845 3.616055 -0.759618
H 2.052607 3.120392 -1.481668
C 5.254330 1.838224 0.315536
H 4.265670 -0.073097 0.437647
C 5.171070 3.167068 -0.114918
H 3.946981 4.650566 -1.104730
H 6.156704 1.478885 0.816213
H 6.007952 3.850066 0.049402
C -2.717586 1.506518 -1.020287
C -2.771185 2.649179 -0.188138
C -3.534786 1.443252 -2.168700
C -3.641400 3.693409 -0.556728
C -4.387625 2.488575 -2.511166
C -4.438385 3.624403 -1.696911
H -3.690520 4.582540 0.078006
H -5.012408 2.415099 -3.404272
H -5.103521 4.454202 -1.948254
C -2.737891 -1.403875 -0.767748
C -4.071128 -1.300476 -0.335689
C -2.219161 -2.671548 -1.089743
C -4.873500 -2.441238 -0.246517
H -4.489445 -0.327085 -0.070769
C -3.027487 -3.807709 -1.004287
H -1.180153 -2.786641 -1.407345
C -4.356240 -3.695564 -0.582666
H -5.909846 -2.346779 0.086935
H -2.615748 -4.784984 -1.267916
H -4.987015 -4.585190 -0.515356
C 1.537631 1.048588 2.346337
C 0.469821 0.846566 3.292847
C 0.630983 -0.125805 4.465957
C -0.673006 -0.841778 4.847170
C -1.202543 -1.733188 3.712408
C -1.584489 -0.978729 2.425964
H 2.451122 0.452447 2.461413
H 1.727856 2.055509 1.961716
H -0.108393 1.745705 3.559961
H -0.620107 0.141567 2.759395
H 1.394946 -0.878077 4.204146
H 1.028416 0.434436 5.329016
H -1.440138 -0.092574 5.118599
H -0.505104 -1.452671 5.748602
H -0.431313 -2.486903 3.473664
H -2.078483 -2.303744 4.068459
H -1.776086 -1.695575 1.615873
H -2.513502 -0.400534 2.568279
H 3.382399 -0.175636 -2.874006
H -3.511998 0.550665 -2.798453
C 1.347540 -2.832878 0.495895
C 2.225889 -2.756588 1.751006
H 0.879186 -3.828290 0.440216
H 0.500818 -2.128146 0.565795
H 3.048766 -3.485542 1.690178
H 2.676087 -1.758616 1.865162
H 1.645644 -2.979437 2.659443
C -1.913035 2.857398 1.042442
C -0.569192 3.528723 0.728246
H -1.753992 1.903722 1.570939
H -2.466939 3.491284 1.752934
H 0.006494 3.720674 1.646815
H 0.052753 2.905137 0.067157
H -0.724418 4.492072 0.217816

^{4}TS5-6C-12
Geometry with 83 atoms:
Total energy: -3124.183390380
Cr -0.268118 -0.993565 0.978857
P 1.448191 0.159992 -0.414038
P -1.705619 0.195934 -0.733419
C -0.646744 0.232626 -2.266047
C 0.687718 0.915214 -1.953132
H -0.484305 -0.817001 -2.561615
H -1.167810 0.726481 -3.099777
H 1.381895 0.814858 -2.798796
H 0.543968 1.991690 -1.779017
C 2.664536 -1.066046 -1.045419
C 3.756442 -0.760062 -1.897073
C 2.404205 -2.407457 -0.698067
C 4.534297 -1.832168 -2.369419
C 3.192660 -3.451360 -1.177336
C 4.264746 -3.156388 -2.023046
H 5.373692 -1.618777 -3.036110
H 2.971387 -4.482947 -0.894345
H 4.893060 -3.959469 -2.416224
C 2.344902 1.499403 0.451888
C 1.723857 2.746760 0.641381
C 3.580671 1.246569 1.070523
C 2.343361 3.730438 1.416290
H 0.748167 2.961368 0.199429
C 4.195196 2.234486 1.844456
H 4.069488 0.278183 0.945147
C 3.580779 3.478614 2.017388
H 1.852436 4.697421 1.551412
H 5.160282 2.029029 2.314095
H 4.064072 4.249540 2.622307
C -2.049270 1.984204 -0.417359
C -1.907202 2.581452 0.858027
C -2.466220 2.768615 -1.510157
C -2.174094 3.956659 0.980333
C -2.725000 4.130471 -1.365167
C -2.572731 4.728142 -0.110859
H -2.063509 4.427008 1.960948
H -3.046133 4.720465 -2.226698
H -2.769413 5.795237 0.019044
C -3.315645 -0.495313 -1.266294
C -4.510757 -0.026158 -0.693280
C -3.365295 -1.567593 -2.174978
C -5.731694 -0.615804 -1.029697
H -4.493369 0.810193 0.008809
C -4.590471 -2.149418 -2.512116
H -2.451283 -1.955351 -2.631169
C -5.775113 -1.676528 -1.939797
H -6.654329 -0.239558 -0.581045
H -4.617793 -2.976124 -3.226209
H -6.731768 -2.133750 -2.203669
C 1.255515 -0.977273 2.441145
C 0.225850 -1.835032 2.975489
C 0.467680 -3.341881 3.117414
C -0.789861 -4.190933 2.883075
C -1.345883 -4.035497 1.459001
C -1.827171 -2.614560 1.114359
H 2.203773 -1.435257 2.135908
H 1.374311 0.029445 2.857375
H -0.368273 -1.413881 3.802281
H -0.888960 -1.993740 2.120992
H 1.249848 -3.648041 2.399686
H 0.879592 -3.535834 4.122283
H -1.568731 -3.908691 3.615529
H -0.555482 -5.250471 3.074724
H -0.559422 -4.338779 0.741906
H -2.176647 -4.747437 1.307414
H -2.069145 -2.552020 0.043855
H -2.751681 -2.361258 1.660395
H 1.567631 -2.635781 -0.030475
H -2.602412 2.309172 -2.491809
C 4.131257 0.644624 -2.336145
C 5.556579 1.061683 -1.950312
H 3.431817 1.382500 -1.924155

H 4.026278 0.701450 -3.434317
H 5.695377 1.040371 -0.858776
H 6.315742 0.403101 -2.399565
H 5.760661 2.087471 -2.295355
C -1.525983 1.808281 2.101400
C -2.674561 0.968527 2.675644
H -1.172424 2.515552 2.867166
H -0.649214 1.171540 1.885823
H -3.520221 1.612097 2.964823
H -3.053768 0.238121 1.943258
H -2.350461 0.414777 3.571134

^{4}TS5-6C-13
Geometry with 83 atoms:
Total energy: -3124.184780920
Cr 0.115222 -0.651016 1.061047
P 1.523201 0.445677 -0.663226
P -1.613671 -0.031861 -0.741929
C -0.682371 -0.032506 -2.353487
C 0.595311 0.803857 -2.259361
H -0.444913 -1.090079 -2.545891
H -1.327161 0.291018 -3.184175
H 1.264950 0.601860 -3.108119
H 0.363187 1.877947 -2.281705
C 3.027069 -0.452620 -1.236930
C 3.220047 -1.841942 -1.044264
C 3.993985 0.292897 -1.943466
C 4.403671 -2.419786 -1.541185
C 5.152915 -0.304919 -2.432216
C 5.362088 -1.671091 -2.220705
H 4.567825 -3.490363 -1.389440
H 5.891022 0.294280 -2.970442
H 6.270763 -2.153663 -2.588826
C 2.080718 2.092636 -0.065488
C 1.158449 3.155140 -0.053049
C 3.333922 2.270878 0.545460
C 1.491639 4.375586 0.539904
H 0.166612 3.039102 -0.494198
C 3.663010 3.494914 1.134325
H 4.059178 1.455595 0.567080
C 2.745214 4.549845 1.133575
H 0.763325 5.190243 0.537891
H 4.643859 3.621906 1.599094
H 3.005844 5.504374 1.597118
C -2.283175 1.680906 -0.578217
C -2.722167 2.165729 0.677589
C -2.363655 2.517294 -1.708518
C -3.195410 3.486433 0.755715
C -2.832986 3.826415 -1.606190
C -3.245840 4.315728 -0.363977
H -3.536620 3.865358 1.723162
H -2.882596 4.457988 -2.496203
H -3.618436 5.338688 -0.270364
C -3.065207 -1.097259 -1.090617
C -4.383711 -0.642664 -0.931968
C -2.840139 -2.428689 -1.489625
C -5.457471 -1.504285 -1.178108
H -4.578433 0.387111 -0.625603
C -3.915652 -3.282255 -1.740841
H -1.820694 -2.806018 -1.607664
C -5.227370 -2.821522 -1.583990
H -6.480158 -1.139076 -1.056301
H -3.728683 -4.311623 -2.056223
H -6.069152 -3.490500 -1.778281
C 1.808081 -0.231497 2.264542
C 0.955462 -1.054843 3.086924
C 1.367771 -2.483112 3.458040
C 0.176350 -3.440114 3.606650
C -0.621800 -3.596916 2.303031
C -1.270404 -2.297504 1.794675
H 2.755694 -0.657495 1.913034
H 1.870120 0.838450 2.487793
H 0.441822 -0.530656 3.907861
H -0.226204 -1.438224 2.466944
H 2.053649 -2.872356 2.685788
H 1.947547 -2.445074 4.395879
H -0.494123 -3.072596 4.405675
H 0.539660 -4.426129 3.938540
H 0.054127 -3.997609 1.524856
H -1.404634 -4.364000 2.441365
H -1.724612 -2.464632 0.811241
H -2.082890 -1.975762 2.469031
H 3.842868 1.362861 -2.104089
H -2.064437 2.150118 -2.690698
C 2.204709 -2.773713 -0.415753
C 1.290729 -3.448672 -1.445114
H 1.586060 -2.238404 0.324575
H 2.735130 -3.547848 0.160957
H 1.874656 -4.054192 -2.155245
H 0.562009 -4.112230 -0.952456
H 0.735574 -2.702433 -2.034523
C -2.676470 1.346442 1.950499
C -1.452975 1.680970 2.813537
H -2.694518 0.269854 1.721303
H -3.592047 1.541986 2.531714
H -1.417974 1.054712 3.718150
H -0.511901 1.540706 2.254751
H -1.469580 2.735407 3.130454

^{4}TS5-6C-14
Geometry with 83 atoms:
Total energy: -3124.183625200
Cr 0.025035 -0.229479 1.230889
P 1.633608 0.323923 -0.633163
P -1.582911 0.128337 -0.744527
C -0.557787 0.125829 -2.302639
C 0.666883 1.013631 -2.072853
H -0.246849 -0.907298 -2.522509
H -1.163895 0.479856 -3.149999
H 1.309121 1.059490 -2.965070
H 0.355441 2.042595 -1.834484
C 2.542195 -1.061667 -1.457365
C 2.274452 -2.428690 -1.217803
C 3.491236 -0.700671 -2.437195
C 2.972692 -3.385812 -1.978928
C 4.173456 -1.665497 -3.173309
C 3.908144 -3.019472 -2.943464
H 2.771031 -4.445908 -1.800767
H 4.906229 -1.362199 -3.924576
H 4.430604 -3.789261 -3.516723
C 2.922028 1.570143 -0.251670
C 2.646353 2.945822 -0.334526
C 4.160565 1.151530 0.266508
C 3.597146 3.882410 0.082750
H 1.691146 3.305469 -0.722329
C 5.106212 2.090879 0.682341
H 4.394269 0.086689 0.338568
C 4.827592 3.458505 0.591967
H 3.373111 4.949255 0.006294
H 6.066501 1.751554 1.078314
H 5.568940 4.192077 0.917599
C -2.489855 1.731849 -0.931172
C -2.233635 2.881217 -0.147966
C -3.429733 1.801276 -1.981260
C -2.942118 4.059747 -0.451651
C -4.121557 2.977370 -2.258020
C -3.873389 4.116430 -1.485872
H -2.749687 4.954597 0.146906
H -4.847360 3.005124 -3.074117
H -4.403387 5.049521 -1.692488
C -2.860157 -1.165527 -0.967154
C -4.121079 -1.008764 -0.364190
C -2.550754 -2.383539 -1.597780
C -5.058491 -2.042750 -0.409057
H -4.377733 -0.071907 0.135872
C -3.493639 -3.414917 -1.640935
H -1.574469 -2.543365 -2.060774
C -4.748320 -3.247616 -1.048037
H -6.037101 -1.905025 0.057310
H -3.244665 -4.352838 -2.143444
H -5.483801 -4.054907 -1.083607
C 1.593775 0.409760 2.486134
C 0.526179 0.039730 3.381160
C 0.648417 -1.166038 4.317737
C -0.697837 -1.857211 4.579961
C -1.299711 -2.466647 3.303801
C -1.613564 -1.456891 2.183760
H 2.490446 -0.220748 2.452003
H 1.810662 1.472881 2.335604
H -0.014830 0.879119 3.844120
H -0.588303 -0.485616 2.729306
H 1.355364 -1.893424 3.882754
H 1.096760 -0.824634 5.266016
H -1.406843 -1.127533 5.013860
H -0.565430 -2.646911 5.336890
H -0.595879 -3.224661 2.917428
H -2.221606 -3.018892 3.558241
H -1.824389 -1.996414 1.250288
H -2.514301 -0.866259 2.422217
H 3.706721 0.354788 -2.620118
H -3.628539 0.914638 -2.588039
C 1.341243 -2.942573 -0.142138
C 2.084821 -3.279895 1.156724
H 0.825649 -3.844065 -0.510237
H 0.532797 -2.214187 0.054070
H 2.592744 -2.394926 1.570364
H 1.397568 -3.675339 1.919644
H 2.856085 -4.043714 0.971984
C -1.297204 2.921913 1.041997
C -2.011918 2.589167 2.358578
H -0.859275 3.930188 1.114472
H -0.438282 2.245044 0.894597
H -2.855456 3.276810 2.525710
H -2.418442 1.565371 2.345788
H -1.327806 2.680346 3.216482

^{4}TS5-6C-15
Geometry with 83 atoms:
Total energy: -3124.183338790
Cr 0.128376 -1.124934 0.805649
P -1.547205 -0.214524 -0.806416
P 1.495262 0.306984 -0.724600
C 0.663941 0.480937 -2.408778
C -0.685299 -0.248515 -2.457965
H 0.519725 1.555640 -2.585500
H 1.345346 0.107839 -3.186994
H -1.335392 0.150000 -3.250639
H -0.553647 -1.318421 -2.682810
C -1.956815 1.561342 -0.510349
C -2.076683 2.089176 0.799325
C -2.140778 2.412142 -1.617267
C -2.362072 3.457326 0.941253
C -2.420872 3.767647 -1.450945
C -2.527502 4.293863 -0.161656
H -2.450050 3.873512 1.948374
H -2.554493 4.408005 -2.325839
H -2.739881 5.355592 -0.014510
C -3.148820 -1.033026 -1.168744
C -3.134668 -2.361538 -1.631172
C -4.380701 -0.384465 -0.986016
C -4.330545 -3.025478 -1.909907
H -2.187208 -2.887031 -1.776752
C -5.576651 -1.057260 -1.256562
H -4.411670 0.649313 -0.637222
C -5.554968 -2.375547 -1.718643
H -4.306993 -4.055938 -2.272673
H -6.529554 -0.543191 -1.108716
H -6.490949 -2.897948 -1.930893
C 3.173052 -0.383792 -1.062339
C 3.303163 -1.716059 -1.526267
C 4.326528 0.383581 -0.817956
C 4.593024 -2.210227 -1.777167
C 5.598760 -0.138362 -1.056161
C 5.732249 -1.437610 -1.549875
H 4.702333 -3.230394 -2.155387
H 6.481858 0.474207 -0.859941
H 6.722502 -1.852513 -1.753043
C 1.742296 2.040095 -0.176327
C 1.381433 2.415675 1.127609
C 2.245476 3.017317 -1.055058
C 1.522435 3.741643 1.547039
H 0.978531 1.677827 1.823538
C 2.382997 4.340989 -0.634345
H 2.538770 2.745466 -2.072117
C 2.021333 4.705398 0.667700
H 1.233961 4.020811 2.563188
H 2.774873 5.091116 -1.325552
H 2.128225 5.742579 0.994588
C -1.371623 -2.519410 1.316975
C -0.313692 -2.742927 2.268837
C -0.461888 -2.282374 3.722907
C 0.868295 -1.879807 4.376778
C 1.565590 -0.710214 3.662661

C	1.953975	-1.014045	2.206412
H	-2.302746	-2.054036	1.658529
H	-1.520836	-3.261195	0.524643
H	0.230807	-3.695805	2.170607
H	0.839650	-2.000224	2.005816
H	-1.159360	-1.426492	3.760664
H	-0.940117	-3.091658	4.300799
H	1.548063	-2.751718	4.389539
H	0.688257	-1.614665	5.431125
H	0.901135	0.174386	3.695979
H	2.468446	-0.422937	4.231079
H	2.460403	-0.153925	1.751199
H	2.680397	-1.844814	2.163854
H	-2.071023	2.018502	-2.632504
H	4.237494	1.401991	-0.438265
C	-1.969465	1.255132	2.058049
C	-3.289360	0.591622	2.468329
H	-1.608061	1.893675	2.879324
H	-1.200993	0.471376	1.932513
H	-3.657954	-0.091466	1.688588
H	-3.167199	0.013422	3.397534
H	-4.069104	1.349903	2.641515
C	2.127342	-2.655120	-1.723868
C	2.129331	-3.840947	-0.748721
H	2.131535	-3.033561	-2.760396
H	1.174853	-2.114965	-1.612953
H	1.236843	-4.470909	-0.893401
H	3.015285	-4.477914	-0.891114
H	2.143156	-3.494900	0.297166

^{4}TS5-6C-16
Geometry with 83 atoms:
Total energy: -3124.182748100

Cr	0.351859	-0.797433	0.892988
P	1.501863	0.850694	-0.523082
P	-1.516760	-0.066153	-0.700259
C	-0.744926	0.877782	-2.138091
C	0.769242	0.660881	-2.230104
H	-1.246532	0.587158	-3.072717
H	-0.960111	1.942121	-1.965683
H	1.007784	-0.351461	-2.588218
H	1.230558	1.369892	-2.935259
C	3.324939	0.677385	-0.678336
C	3.894208	-0.583189	-1.004727
C	4.161323	1.764124	-0.369302
C	5.293195	-0.685111	-1.032144
C	5.550779	1.633932	-0.404280
C	6.116971	0.405467	-0.743052
H	5.757451	-1.640721	-1.280248
H	6.183294	2.490829	-0.161040
H	7.202826	0.287306	-0.774218
C	1.111057	2.605863	-0.162822
C	1.451318	3.629588	-1.067461
C	0.352522	2.925117	0.974459
C	1.047027	4.943857	-0.829137
H	2.034910	3.403392	-1.963023
C	-0.057588	4.241368	1.207429
H	0.065659	2.142845	1.678647
C	0.290186	5.251507	0.307956
H	1.319597	5.731363	-1.535890
H	-0.656469	4.473430	2.091130
H	-0.030949	6.280324	0.487998
C	-2.802391	1.092898	-0.064768
C	-3.041250	1.308714	1.313203
C	-3.552325	1.806233	-1.021773
C	-4.008287	2.264306	1.674948
C	-4.510996	2.741298	-0.638298
C	-4.732408	2.977877	0.721329
H	-4.196589	2.444188	2.737031
H	-5.079923	3.282861	-1.397585
H	-5.474230	3.714554	1.039194
C	-2.451787	-1.420003	-1.511351
C	-3.751996	-1.762934	-1.108760
C	-1.806098	-2.198615	-2.489359
C	-4.397719	-2.862376	-1.683367
H	-4.269534	-1.166904	-0.354265
C	-2.457486	-3.292069	-3.063969
H	-0.787849	-1.954469	-2.807478
C	-3.754561	-3.627437	-2.660161
H	-5.412498	-3.117189	-1.367922
H	-1.950243	-3.885466	-3.828693
H	-4.263134	-4.484254	-3.108502
C	1.766766	-0.249461	2.352073
C	1.085612	-1.400278	2.894743
C	1.827696	-2.731319	3.060286
C	0.950827	-3.965095	2.803603
C	0.425103	-4.015865	1.360458
C	-0.514476	-2.855076	0.987137
H	2.809454	-0.367824	2.033539
H	1.556109	0.738453	2.778049
H	0.378619	-1.196785	3.714572
H	0.103429	-1.953062	2.028056
H	2.685921	-2.748641	2.365195
H	2.253413	-2.767870	4.077350
H	0.098639	-3.969042	3.508819
H	1.532385	-4.876193	3.017892
H	1.292631	-4.021734	0.675671
H	-0.097114	-4.974015	1.190123
H	-0.707607	-2.859896	-0.095801
H	-1.492602	-2.959663	1.482773
H	3.729302	2.724647	-0.086103
H	-3.390497	1.626700	-2.087281
C	3.036272	-1.796489	-1.323609
C	3.637307	-3.161836	-0.990364
H	2.766971	-1.773764	-2.395164
H	2.073781	-1.700364	-0.787090
H	2.897109	-3.957149	-1.168099
H	4.512651	-3.393400	-1.615689
H	3.952229	-3.216624	0.063843
C	-2.386894	0.511192	2.421273
C	-3.123789	-0.801538	2.712092
H	-2.351101	1.124678	3.335323
H	-1.332726	0.290554	2.175879
H	-2.623233	-1.370482	3.511595
H	-4.158884	-0.604151	3.031901
H	-3.168295	-1.438096	1.815264

^{4}TS5-6C-17
Geometry with 83 atoms:
Total energy: -3124.183399900

Cr	-0.052295	0.106697	1.187984
P	1.608486	0.260072	-0.669764
P	-1.559072	-0.054097	-0.790138
C	-0.667005	0.498358	-2.334441
C	0.773345	-0.023581	-2.319749
H	-1.206100	0.149506	-3.227115
H	-0.709720	1.596000	-2.354420
H	0.784118	-1.116504	-2.461521
H	1.377419	0.410295	-3.132102
C	3.046956	-0.891891	-0.700970
C	3.059387	-2.117736	0.005704
C	4.166461	-0.523604	-1.476277
C	4.224855	-2.904889	-0.057515
C	5.298695	-1.331337	-1.539593
C	5.331744	-2.525338	-0.812598
H	4.254534	-3.844335	0.501358
H	6.154629	-1.025013	-2.145500
H	6.219941	-3.161566	-0.836494
C	2.360061	1.936270	-0.787236
C	1.846010	2.921096	-1.647119
C	3.434118	2.271666	0.059836
C	2.381585	4.213610	-1.648904
H	1.026453	2.698706	-2.330502
C	3.968615	3.560805	0.052128
H	3.870456	1.515998	0.715436
C	3.439665	4.538775	-0.797444
H	1.969949	4.965812	-2.326339
H	4.806533	3.801054	0.711095
H	3.857525	5.548302	-0.800674
C	-3.031663	1.047297	-0.661848
C	-2.853272	2.409681	-0.311866
C	-4.329966	0.541490	-0.855497
C	-3.992622	3.225881	-0.226245
C	-5.447051	1.369994	-0.743659
C	-5.275949	2.722171	-0.439952
H	-3.866707	4.282911	0.023656
H	-6.446878	0.957354	-0.897530
H	-6.141573	3.384582	-0.362497
C	-2.162588	-1.729317	-1.241972
C	-1.964365	-2.803235	-0.359531
C	-2.792438	-1.971674	-2.478336
C	-2.388165	-4.091322	-0.700464
H	-1.472064	-2.641055	0.599586
C	-3.213774	-3.258321	-2.817023
H	-2.968258	-1.153368	-3.180442
C	-3.012803	-4.320831	-1.928127
H	-2.223694	-4.917154	-0.004456
H	-3.702492	-3.432674	-3.778681
H	-3.342555	-5.327695	-2.195582
C	1.636153	0.638558	2.355647
C	0.562070	0.446912	3.297551
C	0.526580	-0.781292	4.213268
C	-0.898255	-1.197001	4.606709
C	-1.769034	-1.589399	3.401646
C	-1.967802	-0.462780	2.373354
H	2.444194	-0.102524	2.324513
H	1.965315	1.664544	2.165153
H	0.198443	1.361430	3.793617
H	-0.661601	0.202903	2.714304
H	1.028828	-1.624303	3.705614
H	1.124416	-0.565179	5.115063
H	-1.383434	-0.363961	5.147986
H	-0.850638	-2.038875	5.316120
H	-1.312595	-2.469147	2.908935
H	-2.754929	-1.933100	3.763095
H	-2.598377	-0.806626	1.544924
H	-2.508904	0.386106	2.827321
H	4.158436	0.418321	-2.028508
H	-4.477463	-0.512589	-1.093331
C	1.889110	-2.679012	0.789137
C	1.265702	-3.917611	0.135435
H	1.106129	-1.911494	0.919614
H	2.228473	-2.934228	1.807083
H	2.010044	-4.719844	0.015089
H	0.444175	-4.314549	0.751255
H	0.860733	-3.685546	-0.861545
C	-1.505506	3.028168	0.015867
C	-1.385368	3.503710	1.469953
H	-1.318491	3.879419	-0.660627
H	-0.687074	2.318532	-0.183364
H	-1.593254	2.684644	2.176788
H	-0.372031	3.887181	1.669834
H	-2.098970	4.311725	1.691483

^{4}TS5-6C-18
Geometry with 83 atoms:
Total energy: -3124.183003000

Cr	0.321167	-0.860722	0.947781
P	1.554259	0.734247	-0.462355
P	-1.495663	-0.053705	-0.676448
C	-0.645707	0.782359	-2.139643
C	0.857227	0.485255	-2.175674
H	-1.136817	0.460554	-3.069486
H	-0.809953	1.863920	-2.033613
H	1.046742	-0.560074	-2.460501
H	1.373521	1.121653	-2.911097
C	3.377575	0.522018	-0.562335
C	3.931502	-0.762453	-0.790181
C	4.230326	1.610183	-0.298091
C	5.328773	-0.897876	-0.770185
C	5.616092	1.448667	-0.284043
C	6.168406	0.188786	-0.524898
H	5.764496	-1.886315	-0.941404
H	6.260088	2.306619	-0.077299
H	7.251943	0.048480	-0.510884
C	1.200692	2.510134	-0.176275
C	1.540334	3.485843	-1.132696
C	0.479225	2.894105	0.964656
C	1.167487	4.817220	-0.942892
H	2.098583	3.208455	-2.030214
C	0.101831	4.227509	1.149901
H	0.196241	2.148593	1.709306
C	0.445486	5.189500	0.197658
H	1.438026	5.567606	-1.689680
H	-0.469437	4.510130	2.037105
H	0.148815	6.231523	0.339865
C	-2.665131	1.222430	-0.035412
C	-2.941029	1.391881	1.343335
C	-3.294157	2.061914	-0.976440
C	-3.819071	2.423717	1.720849
C	-4.164439	3.074272	-0.577582
C	-4.421162	3.261144	0.782937
H	-4.033098	2.566492	2.783625

H	-4.637686	3.713399	-1.326592
H	-5.094260	4.055912	1.113629
C	-2.562764	-1.322229	-1.464536
C	-3.927140	-1.447655	-1.160622
C	-1.968015	-2.242712	-2.347496
C	-4.683117	-2.474321	-1.735950
H	-4.407396	-0.737870	-0.484563
C	-2.727980	-3.262024	-2.924022
H	-0.903631	-2.166777	-2.590455
C	-4.088017	-3.381252	-2.616783
H	-5.746025	-2.559520	-1.496839
H	-2.256871	-3.967170	-3.613146
H	-4.682493	-4.180452	-3.065806
C	1.711518	-0.352579	2.444568
C	1.008299	-1.504180	2.955801
C	1.732434	-2.847328	3.104698
C	0.847497	-4.066394	2.808047
C	0.337405	-4.080030	1.358653
C	-0.587724	-2.901951	1.006252
H	2.759256	-0.475426	2.145235
H	1.500190	0.630980	2.880468
H	0.291323	-1.308303	3.768694
H	0.027076	-2.024786	2.065259
H	2.602607	-2.859420	2.424615
H	2.140242	-2.910534	4.127836
H	-0.013836	-4.078164	3.501911
H	1.417518	-4.987744	3.009124
H	1.210946	-4.079084	0.680323
H	-0.192293	-5.029005	1.161741
H	-0.783861	-2.883188	-0.075571
H	-1.567226	-3.004456	1.499956
H	3.812502	2.596177	-0.091217
H	-3.109509	1.922970	-2.043808
C	3.100059	-1.999779	-1.064348
C	3.141345	-2.461908	-2.526432
H	2.050822	-1.830726	-0.763574
H	3.460022	-2.818809	-0.419589
H	2.498630	-3.344086	-2.678092
H	2.809104	-1.668632	-3.214475
H	4.165963	-2.737872	-2.820639
C	-2.410922	0.484488	2.433324
C	-3.241090	-0.793017	2.608055
H	-2.389831	1.040974	3.383448
H	-1.359252	0.211700	2.235092
H	-4.281978	-0.547160	2.870834
H	-3.263599	-1.388077	1.682573
H	-2.828847	-1.425725	3.410013

^{4}TS5-6C-19
Geometry with 83 atoms:
Total energy: -3124.183944160

Cr	0.040736	-1.076689	0.930690
P	-1.566032	-0.190383	-0.735413
P	1.489691	0.219880	-0.662249
C	0.658225	0.342046	-2.348146
C	-0.693720	-0.378278	-2.370238
H	0.510504	1.411002	-2.552894
H	1.335481	-0.049664	-3.120468
H	-1.326899	-0.025899	-3.198480
H	-0.570665	-1.462631	-2.511614
C	-1.867972	1.619459	-0.565083
C	-1.827053	2.262460	0.695647
C	-2.117367	2.377572	-1.724458
C	-2.016134	3.654032	0.737698
C	-2.304723	3.757069	-1.658345
C	-2.246789	4.398899	-0.418285
H	-1.977097	4.161565	1.705217
H	-2.493946	4.327145	-2.570851
H	-2.383284	5.480948	-0.351030
C	-3.210094	-0.939549	-1.042942
C	-4.403851	-0.242412	-0.797490
C	-3.273033	-2.267301	-1.504170
C	-5.638169	-0.866212	-1.006670
H	-4.375284	0.791857	-0.449188
C	-4.507291	-2.881986	-1.721702
H	-2.355325	-2.830333	-1.696860
C	-5.693266	-2.183492	-1.468972
H	-6.561002	-0.314652	-0.810734
H	-4.543665	-3.911824	-2.085223
H	-6.659109	-2.667277	-1.633477
C	3.109591	-0.616537	-0.952355
C	3.142614	-2.006929	-1.225111
C	4.315757	0.095936	-0.826418
C	4.392656	-2.625538	-1.384329
C	5.546160	-0.542195	-0.990406
C	5.584850	-1.908997	-1.273702
H	4.426479	-3.698754	-1.593251
H	6.471562	0.029863	-0.890486
H	6.542498	-2.419878	-1.399949
C	1.875647	1.961902	-0.230735
C	1.668856	2.410684	1.083678
C	2.343348	2.872971	-1.196242
C	1.923888	3.741108	1.427825
H	1.296617	1.726535	1.846896
C	2.593802	4.202304	-0.850767
H	2.520790	2.547716	-2.224337
C	2.384096	4.639018	0.461894
H	1.755884	4.075971	2.454254
H	2.956068	4.899938	-1.609750
H	2.579420	5.680315	0.729548
C	-1.524332	-2.399143	1.440139
C	-0.471533	-2.682959	2.381711
C	-0.588172	-2.224225	3.838966
C	0.767394	-1.918513	4.492025
C	1.530588	-0.779674	3.795981
C	1.874870	-1.065579	2.324645
H	-2.425494	-1.885022	1.793414
H	-1.727012	-3.128041	0.648444
H	0.023201	-3.661784	2.273742
H	0.710437	-1.994557	2.122876
H	-1.224792	-1.322154	3.880716
H	-1.121028	-3.002342	4.411904
H	1.391523	-2.831258	4.483148
H	0.610918	-1.663344	5.552593
H	0.925809	0.145096	3.864999
H	2.459262	-0.568132	4.356239
H	2.411747	-0.219110	1.879289
H	2.560339	-1.927992	2.246663
H	-2.170781	1.886042	-2.697849
H	4.300388	1.161204	-0.593120
C	-1.661504	1.523524	2.006290
C	-2.979420	0.970938	2.560616
H	-1.201722	2.198353	2.744571
H	-0.942846	0.688212	1.885921
H	-2.819971	0.458324	3.522384
H	-3.702105	1.785101	2.726800
H	-3.440479	0.254577	1.863923
C	1.898866	-2.859830	-1.373895
C	1.561851	-3.215152	-2.826942
H	1.034024	-2.353451	-0.903786
H	2.035274	-3.790789	-0.798651
H	0.641194	-3.818220	-2.883355
H	1.424006	-2.315355	-3.445547
H	2.374715	-3.801778	-3.282546

^{4}TS5-6C-20
Geometry with 83 atoms:
Total energy: -3124.185054160

Cr	0.041546	-0.067768	1.223061
P	1.610620	0.275503	-0.691936
P	-1.659026	0.033081	-0.708761
C	-0.749896	0.629368	-2.224891
C	0.689949	0.115177	-2.311327
H	-1.330076	0.377662	-3.126594
H	-0.776799	1.725726	-2.142932
H	0.713338	-0.960186	-2.543375
H	1.250364	0.621790	-3.112881
C	2.998570	-0.922463	-0.899481
C	3.000193	-2.198457	-0.285050
C	4.055641	-0.559639	-1.757630
C	4.079537	-3.059438	-0.553120
C	5.110912	-1.433735	-2.010970
C	5.123235	-2.690919	-1.400800
H	4.094635	-4.045265	-0.080168
H	5.921198	-1.131679	-2.678582
H	5.947217	-3.384950	-1.584013
C	2.409964	1.929407	-0.743364
C	1.879859	2.988502	-1.499220
C	3.538907	2.169749	0.062546
C	2.462122	4.259462	-1.445816
H	1.011769	2.841706	-2.142997
C	4.119983	3.437641	0.108859
H	3.977987	1.358606	0.646378
C	3.580842	4.488300	-0.641643
H	2.039230	5.071053	-2.042967
H	5.001138	3.604831	0.733045
H	4.035993	5.480838	-0.603327
C	-3.044293	1.253109	-0.609981
C	-2.814674	2.539379	-0.065643
C	-4.307517	0.938959	-1.146121
C	-3.873909	3.462646	-0.068887
C	-5.344997	1.870743	-1.130566
C	-5.127328	3.139310	-0.586972
H	-3.703770	4.460607	0.344850
H	-6.318289	1.606801	-1.550912
H	-5.931105	3.879585	-0.573801
C	-2.444113	-1.559590	-1.168270
C	-3.387039	-2.121814	-0.285199
C	-2.086003	-2.276147	-2.322206
C	-3.955152	-3.368118	-0.552992
H	-3.695991	-1.575245	0.608141
C	-2.651264	-3.528662	-2.582427
H	-1.364449	-1.872255	-3.033519
C	-3.583914	-4.078447	-1.699710
H	-4.691659	-3.785429	0.137927
H	-2.362046	-4.073197	-3.484523
H	-4.025968	-5.055989	-1.906632
C	1.537693	0.900258	2.348412
C	0.597337	0.411833	3.326165
C	0.992117	-0.711167	4.291302
C	-0.173012	-1.644868	4.648918
C	-0.716864	-2.392835	3.421809
C	-1.308844	-1.486204	2.327074
H	2.530159	0.435279	2.315572
H	1.550595	1.969902	2.111460
H	-0.048648	1.171983	3.791026
H	-0.467399	-0.318845	2.766538
H	1.806285	-1.304219	3.838279
H	1.411430	-0.253847	5.203444
H	-0.985100	-1.059078	5.118156
H	0.160110	-2.372590	5.406176
H	0.103438	-2.993760	2.989573
H	-1.484217	-3.119495	3.742324
H	-1.475560	-2.070762	1.412228
H	-2.281792	-1.068670	2.636049
H	4.058957	0.425600	-2.228900
H	-4.486225	-0.042605	-1.587110
C	1.878576	-2.718848	0.588634
C	0.743799	-3.374995	-0.205866
H	1.475928	-1.900295	1.213408
H	2.290854	-3.446601	1.304930
H	1.123491	-4.210747	-0.813733
H	-0.037253	-3.768964	0.462782
H	0.263713	-2.661327	-0.890931
C	-1.496081	2.973595	0.542618
C	-1.558111	3.092263	2.070787
H	-1.203797	3.946790	0.114212
H	-0.686128	2.280358	0.259118
H	-2.294599	3.850800	2.376999
H	-1.864108	2.139547	2.531654
H	-0.581217	3.384092	2.486759

^{4}TS5-6C-21
Geometry with 83 atoms:
Total energy: -3124.183555750

Cr	-0.011955	-0.025501	1.244013
P	-1.622730	-0.283306	-0.671219
P	1.592977	-0.020937	-0.753494
C	0.574887	0.065352	-2.313400
C	-0.639187	-0.851702	-2.154042
H	0.249775	1.105985	-2.468711
H	1.193184	-0.222474	-3.176959
H	-1.272843	-0.846153	-3.053086
H	-0.322717	-1.892918	-1.983616
C	-2.455235	1.219587	-1.358175
C	-2.267093	2.526456	-0.853017
C	-3.270518	1.023575	-2.492480
C	-2.900837	3.592910	-1.518718
C	-3.891530	2.093516	-3.131234
C	-3.699813	3.389389	-2.641674
H	-2.760051	4.607587	-1.136180
H	-4.519781	1.916764	-4.007300
H	-4.175081	4.240829	-3.134923

C -2.963144 -1.519320 -0.479365
C -4.262671 -1.122688 -0.121212
C -2.665639 -2.891068 -0.564325
C -5.247587 -2.081187 0.132734
H -4.515121 -0.062330 -0.048574
C -3.655222 -3.845231 -0.314790
H -1.659326 -3.229604 -0.822062
C -4.948169 -3.442990 0.034698
H -6.255674 -1.759571 0.405737
H -3.413657 -4.908125 -0.393075
H -5.720928 -4.190211 0.230286
C 2.623111 -1.523252 -1.078304
C 2.422894 -2.765239 -0.434104
C 3.607816 -1.412309 -2.083704
C 3.234461 -3.850224 -0.818605
C 4.399759 -2.498821 -2.443608
C 4.211141 -3.728151 -1.803360
H 3.087126 -4.815274 -0.325644
H 5.158283 -2.387864 -3.222066
H 4.822084 -4.592087 -2.076409
C 2.767917 1.382075 -0.826421
C 2.384520 2.618127 -1.374720
C 4.017572 1.274602 -0.189249
C 3.242885 3.719374 -1.301202
H 1.416231 2.736809 -1.865710
C 4.870499 2.377556 -0.118220
H 4.331754 0.323918 0.247913
C 4.486321 3.602340 -0.674052
H 2.936978 4.672023 -1.740495
H 5.841264 2.278524 0.373583
H 5.156177 4.463803 -0.619064
C -1.519313 -0.971310 2.375626
C -0.500294 -0.626262 3.334014
C -0.742286 0.451480 4.394334
C 0.529871 1.228042 4.764363
C 1.104302 2.015210 3.575819
C 1.542431 1.153396 2.377271
H -2.474388 -0.432588 2.407946
H -1.628282 -2.017925 2.070036
H 0.106089 -1.463557 3.711303
H 0.590762 0.048381 2.768320
H -1.506903 1.155929 4.025828
H -1.169848 -0.031581 5.289271
H 1.292203 0.523911 5.147100
H 0.308147 1.921490 5.591479
H 0.342273 2.739850 3.237525
H 1.962132 2.622117 3.915773
H 1.764359 1.800656 1.518391
H 2.467358 0.596401 2.604820
H -3.429755 0.013412 -2.877584
H 3.761168 -0.455810 -2.589189
C -1.494870 2.845833 0.408854
C -2.382857 2.795187 1.658691
H -1.051045 3.849615 0.315991
H -0.633427 2.162594 0.516522
H -1.818811 3.073831 2.561484
H -3.227212 3.494798 1.559332
H -2.802687 1.788949 1.810355
C 1.424848 -3.009486 0.679112
C 2.067752 -2.977762 2.070834
H 0.953092 -3.993463 0.522777
H 0.597238 -2.281630 0.628666
H 2.887345 -3.709899 2.137682
H 2.493036 -1.986402 2.294635
H 1.332387 -3.225082 2.852062

4TS5-6C-22
Geometry with 83 atoms:
Total energy: -3124.181851720
Cr 0.265793 -1.069454 0.779818
P 1.601834 0.496984 -0.613124
P -1.472120 -0.116029 -0.775561
C -0.593605 0.604134 -2.287212
C 0.896396 0.240353 -2.317232
H -1.104972 0.256185 -3.196495
H -0.707380 1.695971 -2.240096
H 1.039828 -0.819769 -2.573936
H 1.438778 0.835401 -3.068418
C 3.421532 0.243195 -0.679375
C 3.953587 -1.056320 -0.873096
C 4.292198 1.318327 -0.417503
C 5.346880 -1.220272 -0.820960
C 5.673512 1.128241 -0.370591
C 6.203980 -0.147109 -0.576396
H 5.764376 -2.220566 -0.967058
H 6.331067 1.976432 -0.166244
H 7.283843 -0.309406 -0.536668
C 1.305039 2.281683 -0.323612
C 0.651130 2.683470 0.851993
C 1.638814 3.250781 -1.288091
C 0.337705 4.029150 1.064639
H 0.365969 1.943381 1.602417
C 1.324783 4.593642 -1.073724
H 2.147482 2.958409 -2.210133
C 0.673059 4.984292 0.102573
H -0.180669 4.326765 1.978863
H 1.587590 5.339280 -1.827965
H 0.424282 6.035821 0.265274
C -2.489801 1.285618 -0.134514
C -2.694660 1.532827 1.243779
C -3.062304 2.154701 -1.085371
C -3.432932 2.673452 1.609896
C -3.794547 3.274451 -0.698582
C -3.970120 3.541722 0.661817
H -3.589313 2.877148 2.672871
H -4.223755 3.934534 -1.455865
H -4.532642 4.421572 0.983641
C -2.684521 -1.286280 -1.502438
C -2.211237 -2.271965 -2.387104
C -4.042344 -1.274057 -1.149894
C -3.085210 -3.220750 -2.920075
H -1.153157 -2.302876 -2.664925
C -4.913494 -2.231647 -1.681272
H -4.428497 -0.511985 -0.469853
C -4.439355 -3.203472 -2.565755
H -2.708525 -3.977959 -3.612129
H -5.970374 -2.211369 -1.404259
H -5.123312 -3.947486 -2.981055
C -0.991710 -2.752312 0.926298
C 0.093645 -3.016622 1.835238
C -0.134723 -3.021473 3.350627
C 1.064949 -2.499769 4.155573
C 1.410113 -1.037437 3.830300
C 1.851571 -0.799737 2.375139
H -1.983849 -2.539087 1.339054
H -1.027488 -3.289123 -0.028501
H 0.821199 -3.776622 1.507643
H 1.057411 -1.979391 1.887780
H -1.021505 -2.405010 3.580136
H -0.385438 -4.049631 3.662537
H 1.946925 -3.136837 3.957297
H 0.850424 -2.597195 5.232034
H 0.527227 -0.409154 4.053013
H 2.204907 -0.687195 4.512832
H 1.977567 0.276831 2.189466
H 2.828391 -1.268807 2.169504
H 3.891944 2.317273 -0.240106
H -2.939424 1.953275 -2.151692
C 3.102104 -2.277407 -1.154408
C 3.141617 -2.726454 -2.620799
H 2.056512 -2.090599 -0.852348
H 3.446132 -3.106589 -0.513936
H 2.829792 -1.919355 -3.302226
H 4.162254 -3.019819 -2.912202
H 2.481935 -3.593535 -2.786051
C -2.257687 0.605566 2.358188
C -3.337046 -0.423442 2.714924
H -2.010499 1.203495 3.249961
H -1.328335 0.071280 2.095320
H -3.003906 -1.083677 3.530966
H -4.260623 0.079900 3.041032
H -3.590818 -1.051811 1.847266

4TS5-6C-23
Geometry with 83 atoms:
Total energy: -3124.185091540
Cr 0.021675 -0.194625 1.208585
P 1.609434 0.194744 -0.682694
P -1.651582 0.001519 -0.711628
C -0.732395 0.559959 -2.238403
C 0.699383 0.020366 -2.306974
H -1.312647 0.297409 -3.136582
H -0.741947 1.657581 -2.180201
H 0.702818 -1.060598 -2.516454
H 1.274172 0.500658 -3.114693
C 3.022870 -0.972385 -0.878492
C 3.013348 -2.266803 -0.302613
C 4.110684 -0.570913 -1.677961
C 4.111679 -3.108313 -0.552386
C 5.185570 -1.426497 -1.913493
C 5.185546 -2.702547 -1.344247
H 4.118845 -4.108305 -0.110038
H 6.020249 -1.095281 -2.535749
H 6.023863 -3.382527 -1.514668
C 2.365792 1.868999 -0.718169
C 1.851212 2.907204 -1.513048
C 3.439656 2.147769 0.148343
C 2.388770 4.196362 -1.432904
H 1.029521 2.730141 -2.207544
C 3.978572 3.433030 0.219511
H 3.867994 1.353223 0.762095
C 3.450273 4.463827 -0.565707
H 1.976220 4.991539 -2.058604
H 4.816767 3.630152 0.892249
H 3.870122 5.470738 -0.505490
C -2.940985 1.314296 -0.539984
C -2.625946 2.535210 0.115840
C -4.208575 1.134081 -1.117367
C -3.617435 3.525361 0.171970
C -5.179192 2.135588 -1.043679
C -4.881191 3.332559 -0.393851
H -3.405169 4.472574 0.669102
H -6.160130 1.977652 -1.498062
H -5.630354 4.125489 -0.327740
C -2.544366 -1.528158 -1.179588
C -3.546712 -2.017030 -0.319351
C -2.194721 -2.281687 -2.312304
C -4.186990 -3.226459 -0.593203
H -3.841624 -1.441405 0.560635
C -2.833115 -3.497220 -2.578429
H -1.422202 -1.934900 -3.000353
C -3.828484 -3.972642 -1.721240
H -4.969572 -3.587681 0.078385
H -2.551251 -4.071291 -3.464409
H -4.327895 -4.921193 -1.932708
C 1.469692 0.765287 2.395656
C 0.474218 0.296366 3.328773
C 0.814082 -0.808181 4.336108
C -0.350780 -1.768101 4.617971
C -0.798264 -2.526601 3.358781
C -1.359333 -1.626139 2.243543
H 2.457857 0.290015 2.420211
H 1.504782 1.832365 2.151418
H -0.194988 1.066594 3.744416
H -0.557333 -0.454547 2.721488
H 1.673727 -1.386571 3.953809
H 1.153088 -0.332677 5.272059
H -1.205661 -1.202370 5.032839
H -0.049804 -2.487585 5.396251
H 0.064666 -3.096127 2.968334
H -1.557646 -3.280727 3.631090
H -1.486283 -2.206935 1.318973
H -2.348784 -1.224875 2.518396
H 4.122671 0.429487 -2.116066
H -4.446640 0.203518 -1.635455
C 1.863697 -2.818119 0.514972
C 0.737786 -3.420216 -0.334172
H 1.458487 -2.025639 1.173175
H 2.250466 -3.587191 1.201566
H 1.121374 -4.230138 -0.973913
H -0.060348 -3.837796 0.298969
H 0.278064 -2.669884 -0.994338
C -1.258454 2.765897 0.737617
C -0.947000 4.166771 1.256964
H -0.479073 2.501237 0.004286
H -1.137384 2.050678 1.573989
H -1.615708 4.462659 2.080026
H 0.085552 4.201875 1.637622
H -1.030215 4.922172 0.459595

4TS5-6C-24
Geometry with 83 atoms:
Total energy: -3124.184002330

Cr	0.043036	-0.539753	1.147039
P	-1.620042	-0.292329	-0.767087
P	1.596633	0.105589	-0.772438
C	0.650114	0.171194	-2.390147
C	-0.649764	-0.633457	-2.322151
H	0.449636	1.229167	-2.608657
H	1.298867	-0.204531	-3.194275
H	-1.278772	-0.471260	-3.210614
H	-0.439227	-1.713740	-2.292239
C	-2.300936	1.412842	-0.991212
C	-2.933799	2.080089	0.086643
C	-2.184439	2.069250	-2.231831
C	-3.386232	3.394871	-0.111018
C	-2.638817	3.377082	-2.404239
C	-3.234860	4.047865	-1.334023
H	-3.876858	3.911213	0.718908
H	-2.532850	3.865060	-3.375857
H	-3.595516	5.072123	-1.455717
C	-3.052633	-1.428043	-0.949262
C	-2.807163	-2.813485	-0.979633
C	-4.373136	-0.964662	-1.057675
C	-3.862455	-3.715411	-1.124371
H	-1.787606	-3.197900	-0.893604
C	-5.428305	-1.872998	-1.192055
H	-4.585185	0.106079	-1.044777
C	-5.176847	-3.246798	-1.227015
H	-3.657951	-4.788476	-1.152227
H	-6.452201	-1.500372	-1.275328
H	-6.003276	-3.953492	-1.334526
C	3.088000	-0.895228	-1.196468
C	3.373671	-2.159688	-0.628950
C	3.945966	-0.362441	-2.181410
C	4.526821	-2.835274	-1.070164
C	5.081319	-1.051411	-2.600732
C	5.374145	-2.296663	-2.036629
H	4.759547	-3.811882	-0.636973
H	5.734901	-0.616950	-3.360707
H	6.263408	-2.848735	-2.350647
C	2.195807	1.824805	-0.514279
C	3.498391	2.100282	-0.066750
C	1.261942	2.875829	-0.591883
C	3.864783	3.406645	0.272014
H	4.233713	1.298259	0.020464
C	1.633949	4.178190	-0.252572
H	0.232578	2.687890	-0.907374
C	2.937146	4.447663	0.178998
H	4.883230	3.608361	0.612930
H	0.898589	4.983461	-0.323125
H	3.227047	5.466820	0.445839
C	-1.318517	-1.887798	2.024582
C	-0.219916	-1.812628	2.957254
C	-0.389537	-1.207609	4.354507
C	0.877405	-0.500981	4.859015
C	1.253488	0.710788	3.990986
C	1.587069	0.382052	2.523612
H	-2.277005	-1.441094	2.315312
H	-1.432992	-2.791930	1.418763
H	0.457343	-2.681676	2.957990
H	0.745909	-0.881899	2.592589
H	-1.226256	-0.488822	4.338230
H	-0.683676	-2.013674	5.047618
H	1.717138	-1.220502	4.879685
H	0.725385	-0.174040	5.900126
H	0.416785	1.430274	4.019660
H	2.114384	1.233830	4.443424
H	1.613240	1.309244	1.934388
H	2.579930	-0.090927	2.436539
H	-1.743254	1.563470	-3.090302
H	3.726563	0.614250	-2.620188
C	-3.130572	1.450896	1.449098
C	-2.032524	1.842886	2.441764
H	-3.186685	0.355550	1.365948
H	-4.107027	1.768877	1.848264
H	-2.181677	1.355242	3.416794
H	-1.033564	1.560776	2.065748
H	-2.008428	2.931849	2.603381
C	2.479819	-2.861082	0.371717
C	1.332818	-3.641172	-0.284816
H	2.073714	-2.135885	1.092000
H	3.091038	-3.557619	0.966673
H	0.712680	-4.148447	0.471389
H	0.679883	-2.974989	-0.870991
H	1.719560	-4.406183	-0.976024

^{4}TS5-6C-25

Geometry with 83 atoms:

Total energy: -3124.185894760

Cr	0.042581	-0.235317	1.213366
P	1.573537	0.360954	-0.673786
P	-1.678063	0.104651	-0.676940
C	-0.790994	0.778595	-2.177714
C	0.657351	0.299675	-2.300803
H	-1.376085	0.549879	-3.082141
H	-0.840505	1.869895	-2.054389
H	0.700215	-0.755575	-2.611159
H	1.209066	0.873952	-3.061843
C	3.041588	-0.708661	-1.001927
C	3.118708	-2.054896	-0.565910
C	4.090160	-0.163627	-1.769085
C	4.262972	-2.795489	-0.912161
C	5.210781	-0.921952	-2.103493
C	5.298298	-2.246293	-1.667749
H	4.336573	-3.832818	-0.574487
H	6.012611	-0.477276	-2.697522
H	6.173820	-2.851943	-1.914490
C	2.256999	2.064798	-0.562744
C	1.691628	3.142690	-1.264227
C	3.333317	2.314525	0.310306
C	2.182948	4.440768	-1.088730
H	0.867096	2.989958	-1.960599
C	3.825003	3.609768	0.477421
H	3.805112	1.490731	0.848552
C	3.247192	4.678800	-0.216493
H	1.732098	5.266592	-1.644452
H	4.666722	3.784184	1.152076
H	3.632041	5.692634	-0.082930
C	-2.999548	1.374238	-0.452462
C	-2.714449	2.564765	0.258098
C	-4.253752	1.211571	-1.069384
C	-3.713844	3.549034	0.333829
C	-5.231584	2.202164	-0.975272
C	-4.960011	3.376544	-0.269145
H	-3.502259	4.472402	0.880614
H	-6.199934	2.057568	-1.460200
H	-5.716533	4.161442	-0.192483
C	-2.541023	-1.413928	-1.230069
C	-3.543377	-1.959162	-0.404208
C	-2.169734	-2.106323	-2.394479
C	-4.164613	-3.161592	-0.744007
H	-3.852319	-1.434055	0.502440
C	-2.788794	-3.315791	-2.726674
H	-1.395388	-1.716722	-3.057128
C	-3.785816	-3.845848	-1.904248
H	-4.947604	-3.566548	-0.098372
H	-2.490098	-3.842192	-3.636415
H	-4.270376	-4.789180	-2.167249
C	1.620986	0.452230	2.428575
C	0.719177	-0.214906	3.336368
C	1.135100	-1.502815	4.052854
C	-0.037684	-2.465374	4.288282
C	-0.645554	-2.969285	2.970100
C	-1.247078	-1.874301	2.069130
H	2.599697	-0.009206	2.250450
H	1.648483	1.547517	2.422153
H	0.111977	0.444524	3.973963
H	-0.368207	-0.819412	2.698570
H	1.913587	-2.014682	3.460127
H	1.606098	-1.229070	5.012147
H	-0.815702	-1.959207	4.889856
H	0.305745	-3.324205	4.887021
H	0.142546	-3.503624	2.410405
H	-1.422819	-3.723351	3.186213
H	-1.421750	-2.284946	1.065851
H	-2.217943	-1.525178	2.458073
H	4.035000	0.874669	-2.102544
H	-4.472852	0.303483	-1.633527
C	2.023013	-2.765931	0.201120
C	0.891264	-3.300081	-0.685474
H	1.604890	-2.100268	0.975056
H	2.470506	-3.605262	0.755577
H	0.155521	-3.864888	-0.092415
H	0.348600	-2.486960	-1.189118
H	1.284129	-3.969933	-1.466097
C	-1.409213	2.812280	0.987678
C	-1.483869	2.400159	2.462813
H	-1.156258	3.882401	0.921139
H	-0.570365	2.288339	0.497811
H	-1.699732	1.323324	2.564333
H	-0.540797	2.617202	2.987297
H	-2.291964	2.941220	2.979239

^{4}TS5-6C-26

Geometry with 83 atoms:

Total energy: -3124.184430840

Cr	0.067100	-0.819367	1.054618
P	1.516671	0.444263	-0.523590
P	-1.545220	-0.022778	-0.716393
C	-0.634330	-0.015581	-2.338997
C	0.763158	0.608331	-2.246687
H	-0.571001	-1.079823	-2.611190
H	-1.248483	0.462747	-3.117227
H	1.445077	0.154815	-2.979504
H	0.725206	1.683397	-2.466279
C	3.122740	-0.426174	-0.769683
C	3.121887	-1.784529	-1.172505
C	4.337765	0.201589	-0.442836
C	4.353787	-2.450775	-1.271833
C	5.549365	-0.483511	-0.547534
C	5.558403	-1.814160	-0.970791
H	4.361709	-3.499872	-1.581106
H	6.482570	0.023757	-0.291550
H	6.500803	-2.360976	-1.053277
C	1.883954	2.192934	-0.107559
C	2.637106	3.000861	-0.981281
C	1.308700	2.773593	1.032593
C	2.816435	4.357646	-0.707950
H	3.085648	2.569721	-1.880200
C	1.483486	4.134753	1.300158
H	0.701662	2.171800	1.709184
C	2.238709	4.927211	0.433145
H	3.406569	4.974605	-1.389983
H	1.019786	4.574752	2.186081
H	2.375726	5.991086	0.641900
C	-2.014988	1.722876	-0.367024
C	-2.558425	2.071331	0.894386
C	-1.789410	2.726426	-1.327861
C	-2.835005	3.424787	1.148221
C	-2.064681	4.064599	-1.048734
C	-2.585094	4.415868	0.199046
H	-3.263615	3.701710	2.115564
H	-1.876366	4.828340	-1.806596
H	-2.806939	5.460855	0.428939
C	-3.089555	-0.912631	-1.154020
C	-4.355415	-0.309961	-1.092840
C	-2.987895	-2.261692	-1.544546
C	-5.498751	-1.043902	-1.424491
H	-4.453245	0.734896	-0.791198
C	-4.131356	-2.987740	-1.881974
H	-2.011948	-2.755183	-1.584221
C	-5.390035	-2.379774	-1.820319
H	-6.479716	-0.564951	-1.376010
H	-4.040219	-4.032707	-2.188168
H	-6.285827	-2.949110	-2.080004
C	1.773272	-0.577202	2.300302
C	0.935002	-1.535446	2.978351
C	1.331951	-3.015934	2.994416
C	0.131157	-3.972279	3.028478
C	-0.800631	-3.814204	1.815941
C	-1.442378	-2.420790	1.706834
H	2.705826	-0.939909	1.854370
H	1.858831	0.431939	2.718728
H	0.480178	-1.197395	3.923338
H	-0.299819	-1.716852	2.392077
H	1.944708	-3.232194	2.100677
H	1.986996	-3.194869	3.864135
H	-0.448613	-3.796542	3.953439
H	0.495214	-5.010882	3.085038
H	-0.228914	-4.036220	0.894114
H	-1.593572	-4.582500	1.863492
H	-2.109152	-2.362805	0.840863
H	-2.068822	-2.218119	2.593735
H	4.344756	1.234501	-0.093416
H	-1.397419	2.473029	-2.313270

C	1.860571	-2.564078	-1.493115
C	1.658579	-2.841504	-2.987592
H	0.972821	-2.039468	-1.095008
H	1.896127	-3.526060	-0.954382
H	2.496223	-3.430056	-3.393031
H	0.733106	-3.413454	-3.161964
H	1.602917	-1.909758	-3.570932
C	-2.854031	1.060567	1.986406
C	-1.850661	1.105441	3.147522
H	-2.900259	0.040378	1.577042
H	-3.862496	1.263951	2.383041
H	-0.824936	0.874663	2.809358
H	-1.817802	2.104012	3.610532
H	-2.115787	0.375616	3.928012

^{4}TS5-6C-27
Geometry with 83 atoms:
Total energy: -3124.182427260

Cr	0.141804	-0.286150	1.151240
P	1.672072	0.443236	-0.644190
P	-1.497363	0.025355	-0.805461
C	-0.576107	0.788001	-2.242479
C	0.878622	0.320486	-2.336613
H	-1.130951	0.604451	-3.176146
H	-0.615684	1.873763	-2.057768
H	0.956797	-0.719614	-2.678434
H	1.441131	0.933726	-3.055580
C	3.218232	-0.552442	-0.728178
C	3.145237	-1.961015	-0.885300
C	4.469952	0.062391	-0.543004
C	4.347113	-2.686799	-0.907788
C	5.647756	-0.686089	-0.551511
C	5.586983	-2.066867	-0.748141
H	4.302343	-3.771268	-1.043617
H	6.608857	-0.187023	-0.407119
H	6.502458	-2.663157	-0.768069
C	2.137186	2.224848	-0.628020
C	2.940609	2.765005	-1.650980
C	1.614880	3.088471	0.348180
C	3.223567	4.131319	-1.683516
H	3.356307	2.115137	-2.424945
C	1.891305	4.458976	0.308704
H	0.982909	2.700355	1.147511
C	2.698384	4.981926	-0.703869
H	3.854595	4.534511	-2.479231
H	1.474122	5.117152	1.074694
H	2.918078	6.051930	-0.732842
C	-2.974702	1.124012	-0.661431
C	-3.058590	2.171255	0.286467
C	-4.011343	0.949921	-1.602100
C	-4.197098	2.998472	0.257825
C	-5.127756	1.781934	-1.607953
C	-5.220891	2.813189	-0.668138
H	-4.271347	3.815183	0.981327
H	-5.919076	1.628378	-2.345411
H	-6.088808	3.477224	-0.662164
C	-2.168442	-1.566124	-1.432921
C	-3.236976	-2.174279	-0.745721
C	-1.591636	-2.241215	-2.521959
C	-3.711409	-3.426678	-1.139277
H	-3.713939	-1.658838	0.090527
C	-2.066653	-3.498616	-2.909326
H	-0.774143	-1.795882	-3.089202
C	-3.123632	-4.095818	-2.218441
H	-4.546964	-3.880895	-0.601238
H	-1.609153	-4.007831	-3.761133
H	-3.494847	-5.076915	-2.524195
C	1.805064	0.206407	2.372561
C	0.706707	-0.029819	3.283358
C	0.759982	-1.179658	4.299302
C	-0.605576	-1.829683	4.558450
C	-1.160985	-2.504438	3.294815
C	-1.447940	-1.549732	2.119345
H	2.592416	-0.556722	2.320564
H	2.191806	1.223264	2.261350
H	0.240233	0.877669	3.698634
H	-0.413336	-0.559604	2.672020
H	1.462098	-1.947637	3.931072
H	1.189479	-0.788619	5.236698
H	-1.318996	-1.067428	4.923963
H	-0.510424	-2.575510	5.363899
H	-0.432915	-3.267479	2.965821
H	-2.084356	-3.056354	3.543782
H	-1.558280	-2.141680	1.200166
H	-2.387128	-0.994855	2.273558
H	4.532503	1.139101	-0.382343
H	-3.945511	0.147069	-2.339544
C	1.846982	-2.746756	-0.934293
C	1.448099	-3.309910	0.436629
H	1.955835	-3.579424	-1.647866
H	1.015205	-2.139179	-1.316187
H	0.493279	-3.855234	0.377256
H	2.215250	-3.994565	0.829857
H	1.335040	-2.500703	1.179878
C	-2.005708	2.472969	1.335151
C	-2.462119	2.194703	2.771742
H	-1.716211	3.533692	1.244348
H	-1.084447	1.905354	1.127049
H	-1.671756	2.458701	3.492645
H	-3.354984	2.785147	3.028733
H	-2.715993	1.133267	2.913297

^{4}TS5-6C-28
Geometry with 83 atoms:
Total energy: -3124.182913700

Cr	0.131924	-1.063421	0.790395
P	-1.624304	-0.182151	-0.761359
P	1.422978	0.428573	-0.750781
C	0.579080	0.553331	-2.428774
C	-0.807874	-0.109866	-2.437134
H	0.506354	1.621988	-2.669695
H	1.233428	0.098129	-3.185928
H	-1.485126	0.361313	-3.165547
H	-0.729903	-1.167173	-2.733230
C	-2.108510	1.552451	-0.351304
C	-2.622089	1.874875	0.929783
C	-1.920392	2.578666	-1.295897
C	-2.896198	3.221492	1.219146
C	-2.193760	3.910073	-0.982861
C	-2.676910	4.234657	0.285914
H	-3.298315	3.475100	2.204169
H	-2.031888	4.688633	-1.731700
H	-2.894607	5.273633	0.544981
C	-3.185285	-1.070280	-1.151275
C	-3.103636	-2.399444	-1.606051
C	-4.447228	-0.469974	-1.017305
C	-4.261630	-3.110268	-1.925755
H	-2.131471	-2.887919	-1.716196
C	-5.605390	-1.189218	-1.328953
H	-4.532200	0.562519	-0.673090
C	-5.516221	-2.507249	-1.783725
H	-4.184855	-4.140182	-2.282703
H	-6.582064	-0.711528	-1.219098
H	-6.423009	-3.065600	-2.028724
C	3.094544	-0.264658	-1.095569
C	3.207275	-1.587159	-1.593179
C	4.254668	0.478891	-0.815976
C	4.492375	-2.091072	-1.848059
C	5.521643	-0.054470	-1.057498
C	5.639888	-1.339819	-1.589581
H	4.595946	-3.100524	-2.254138
H	6.412006	0.537822	-0.833703
H	6.625796	-1.762880	-1.797046
C	1.648749	2.176212	-0.246707
C	1.189628	2.601687	1.010134
C	2.209256	3.120241	-1.127463
C	1.291603	3.945144	1.383044
H	0.730962	1.892324	1.700717
C	2.308539	4.461008	-0.752642
H	2.574351	2.808934	-2.109732
C	1.849354	4.875424	0.503169
H	0.923539	4.263986	2.360957
H	2.745695	5.186149	-1.443375
H	1.925661	5.926235	0.793106
C	-1.250408	-2.572418	1.321467
C	-0.058064	-2.877884	2.071464
C	-0.017050	-2.749291	3.597705
C	1.371303	-2.369935	4.133195
C	1.852886	-1.001672	3.624011
C	2.017578	-0.911208	2.096389
H	-2.125552	-2.194188	1.863382
H	-1.511786	-3.216443	0.476501
H	0.519901	-3.740749	1.703523
H	0.966802	-1.966108	1.879118
H	-0.752221	-1.990796	3.915156
H	-0.348173	-3.705947	4.036047
H	2.101641	-3.147533	3.841869
H	1.349104	-2.365615	5.234904
H	1.138169	-0.229318	3.962301
H	2.814646	-0.751465	4.106199
H	2.287714	0.114111	1.811559
H	2.839935	-1.556771	1.743977
H	-1.558326	2.351945	-2.298332
H	4.174010	1.485901	-0.404653
C	-2.882303	0.846173	2.012544
C	-1.730498	0.718311	3.014704
H	-3.102630	-0.138278	1.573910
H	-3.794332	1.138631	2.557385
H	-1.981875	0.016675	3.824225
H	-0.815525	0.340850	2.523980
H	-1.478502	1.689936	3.467069
C	2.009847	-2.491837	-1.835336
C	2.065825	-3.816555	-1.064978
H	1.916927	-2.697535	-2.916344
H	1.076033	-1.976525	-1.556073
H	1.143997	-4.398877	-1.224281
H	2.911522	-4.443026	-1.385167
H	2.178390	-3.640224	0.016462

^{4}TS9-10A-01
Geometry with 77 atoms:
Total energy: -3045.582605600

Cr	-0.076188	-0.716797	1.142298
P	1.768536	0.292844	-0.489471
P	-1.487854	0.479521	-0.559978
C	-0.449146	1.063265	-2.012371
C	0.893286	0.327226	-2.133304
H	-1.032325	0.965800	-2.940626
H	-0.279189	2.138253	-1.845758
H	0.740564	-0.720854	-2.437191
H	1.529958	0.804792	-2.894714
C	3.319173	-0.639866	-0.746430
C	3.557666	-1.441314	-1.875408
C	4.268470	-0.625891	0.295081
C	4.724002	-2.210399	-1.959876
H	2.846386	-1.469424	-2.703236
C	5.432494	-1.389509	0.202908
H	4.101442	-0.004042	1.179405
C	5.661591	-2.186851	-0.924653
H	4.901399	-2.825641	-2.845350
H	6.164036	-1.363008	1.014302
H	6.572136	-2.786518	-0.995351
C	2.270333	2.043696	-0.250789
C	3.487613	2.546877	-0.742748
C	1.376610	2.918720	0.393491
C	3.801044	3.899780	-0.589810
H	4.195293	1.881917	-1.242937
C	1.689551	4.273436	0.533502
H	0.427942	2.549818	0.787404
C	2.903655	4.765077	0.045661
H	4.751379	4.280588	-0.972019
H	0.982591	4.942095	1.030582
H	3.152775	5.822690	0.162075
C	-2.710844	-0.681458	-1.276881
C	-4.047155	-0.680857	-0.845772
C	-2.276837	-1.678902	-2.168255
C	-4.932988	-1.659825	-1.304994
H	-4.401607	0.082613	-0.150323
C	-3.166293	-2.653730	-2.625537
H	-1.240456	-1.705114	-2.512339
C	-4.496373	-2.647858	-2.192100
H	-5.971165	-1.649104	-0.964673
H	-2.818766	-3.420666	-3.322001
H	-5.191530	-3.412234	-2.547299
C	-2.430878	1.958153	-0.047323
C	-3.178034	2.696500	-0.983179
C	-2.387146	2.377964	1.291563
C	-3.864061	3.843403	-0.580935
H	-3.229979	2.372854	-2.025897
C	-3.077140	3.527619	1.689699
H	-1.814912	1.805968	2.024031
C	-3.813168	4.260458	0.754884
H	-4.442734	4.413613	-1.311693

H	-3.040126	3.848317	2.733479
H	-4.352733	5.158319	1.066240
C	1.302022	-2.393248	1.721615
C	0.541321	-2.999609	0.528080
C	-0.345986	-4.208941	0.844790
C	-1.436034	-3.977572	1.897335
C	-2.373001	-2.792428	1.611787
C	-1.828742	-1.425569	2.045713
H	2.330315	-2.150598	1.436184
H	1.313587	-3.118798	2.541183
H	-0.110389	-2.291934	-0.073372
H	1.292511	-3.263784	-0.235049
H	-0.820007	-4.536911	-0.096667
H	0.308753	-5.036665	1.167052
H	-0.976083	-3.844655	2.893525
H	-2.026058	-4.906443	1.966460
H	-2.638423	-2.785459	0.539294
H	-3.327747	-2.977668	2.139546
H	-2.609483	-0.656110	1.904011
H	-1.625502	-1.448351	3.132624
C	0.534030	0.333652	2.827235
C	1.109092	-0.929789	3.178910
H	-0.368931	0.642593	3.364423
H	1.217691	1.148110	2.564107
H	2.194778	-0.993141	3.288230
H	0.564143	-1.546818	3.897618

^{4}TS9-10A-02
Geometry with 77 atoms:
Total energy: -3045.579037430

Cr	-0.070479	-0.690795	1.146988
P	1.774345	0.286562	-0.492812
P	-1.470630	0.490031	-0.587434
C	-0.424998	1.073417	-2.033182
C	0.918553	0.337626	-2.145669
H	-1.001983	0.974484	-2.965005
H	-0.254996	2.148403	-1.866653
H	0.772219	-0.706632	-2.464125
H	1.564734	0.823783	-2.893442
C	3.323525	-0.651520	-0.739589
C	3.566674	-1.449825	-1.870000
C	4.264318	-0.647608	0.309672
C	4.729023	-2.225386	-1.948281
H	2.861970	-1.470782	-2.703617
C	5.424632	-1.417686	0.223509
H	4.094922	-0.027965	1.194934
C	5.658331	-2.211643	-0.905438
H	4.909918	-2.837966	-2.834906
H	6.149883	-1.398514	1.040724
H	6.565934	-2.816299	-0.971316
C	2.274869	2.035234	-0.238043
C	3.498947	2.540598	-0.709975
C	1.370015	2.907086	0.395233
C	3.808682	3.893388	-0.548108
H	4.214420	1.877721	-1.201869
C	1.679576	4.261517	0.544133
H	0.415306	2.534240	0.772697
C	2.900753	4.755601	0.076329
H	4.764226	4.276455	-0.914764
H	0.965048	4.928434	1.032591
H	3.146980	5.813094	0.199816
C	-2.670187	-0.693870	-1.313194
C	-4.022138	-0.683493	-0.932913
C	-2.204879	-1.712835	-2.163702
C	-4.891511	-1.673138	-1.401801
H	-4.401947	0.097465	-0.270828
C	-3.077856	-2.697332	-2.631699
H	-1.157180	-1.748269	-2.469539
C	-4.423308	-2.681361	-2.249002
H	-5.941812	-1.653555	-1.101253
H	-2.705253	-3.480635	-3.296286
H	-5.105492	-3.453610	-2.612230
C	-2.436702	1.956984	-0.088101
C	-3.079021	2.763061	-1.045531
C	-2.525863	2.291261	1.272696
C	-3.793979	3.891791	-0.641983
H	-3.025389	2.509439	-2.107419
C	-3.246963	3.421110	1.671856
H	-2.035155	1.666908	2.022000
C	-3.878392	4.221670	0.716226
H	-4.289543	4.515938	-1.389565
H	-3.314612	3.674408	2.732560
H	-4.440409	5.105370	1.028372
C	1.232728	-2.391444	1.730858
C	0.470453	-2.997327	0.529873
C	-0.469056	-4.176245	0.829376
C	-1.878336	-3.804701	1.304131
C	-1.936666	-2.835232	2.495224
C	-1.813683	-1.352914	2.116690
H	2.264977	-2.160833	1.446386
H	1.237040	-3.120303	2.546875
H	-0.134657	-2.274970	-0.099898
H	1.245873	-3.296389	-0.194600
H	-0.556015	-4.781519	-0.088482
H	0.019936	-4.824352	1.577247
H	-2.398694	-4.742157	1.561575
H	-2.443674	-3.367315	0.460955
H	-2.902876	-2.987067	3.012673
H	-1.167595	-3.120371	3.237172
H	-2.684726	-1.086960	1.492487
H	-1.894094	-0.733201	3.027788
C	0.621407	0.363950	2.803008
C	1.052593	-0.943910	3.194026
H	-0.253849	0.784447	3.307777
H	1.392159	1.095499	2.537752
H	2.119688	-1.107350	3.366309
H	0.411229	-1.499836	3.883298

^{4}TS9-10A-03
Geometry with 77 atoms:
Total energy: -3045.573565750

Cr	0.081503	-0.687999	1.086981
P	1.328406	0.778147	-0.655729
P	-1.826246	-0.015282	-0.446506
C	-1.158152	0.924373	-1.921744
C	0.317699	0.620077	-2.209190
H	-1.784570	0.727503	-2.805226
H	-1.284215	1.989937	-1.674288
H	0.447832	-0.412603	-2.569055
H	0.711062	1.298657	-2.982228
C	3.049867	0.373382	-1.106737
C	3.408048	-0.210250	-2.333062
C	4.041118	0.576987	-0.127595
C	4.733834	-0.587220	-2.570579
H	2.664066	-0.379747	-3.113390
C	5.362905	0.202154	-0.371046
H	3.780350	1.037519	0.828873
C	5.711127	-0.385930	-1.592441
H	5.002038	-1.040445	-3.527981
H	6.123274	0.366437	0.396202
H	6.745088	-0.684096	-1.781555
C	1.322726	2.580680	-0.306878
C	2.227274	3.469783	-0.913129
C	0.348156	3.087665	0.570170
C	2.148613	4.838945	-0.647421
H	2.999284	3.093863	-1.588563
C	0.265160	4.458622	0.826611
H	-0.363129	2.412093	1.050574
C	1.167653	5.335845	0.218423
H	2.857303	5.522958	-1.120727
H	-0.503360	4.838745	1.503972
H	1.109793	6.408045	0.421162
C	-2.699432	-1.473246	-1.130039
C	-3.725599	-2.070957	-0.374952
C	-2.303573	-2.068573	-2.339416
C	-4.343643	-3.238762	-0.826619
H	-4.055323	-1.616708	0.562480
C	-2.925414	-3.238348	-2.786242
H	-1.510721	-1.627677	-2.947112
C	-3.943847	-3.826557	-2.031457
H	-5.144466	-3.689618	-0.235504
H	-2.611476	-3.689921	-3.730459
H	-4.429024	-4.740230	-2.383017
C	-3.156586	1.074897	0.188458
C	-4.284346	1.359876	-0.602448
C	-3.036442	1.673047	1.453374
C	-5.268511	2.231789	-0.133594
H	-4.398932	0.891693	-1.583444
C	-4.023230	2.547271	1.919915
H	-2.174481	1.454094	2.087911
C	-5.138952	2.827246	1.126730
H	-6.142623	2.446346	-0.753193
H	-3.921369	3.004554	2.907058
H	-5.912430	3.507340	1.491731
C	1.593216	-0.822715	2.656706
C	2.577967	-1.811453	3.267999
C	3.342101	-2.681901	2.262681
C	2.539575	-3.591299	1.312647
C	1.992205	-2.953709	0.017672
C	0.575116	-2.382043	0.029361
H	2.076855	-0.414139	1.745407
H	1.381681	0.031488	3.321150
H	3.324339	-1.237070	3.846405
H	2.078929	-2.456558	4.013255
H	3.995800	-2.033835	1.650360
H	4.025379	-3.319428	2.848936
H	1.725306	-4.101509	1.859096
H	3.224651	-4.397815	1.004100
H	2.712795	-2.198689	-0.340346
H	2.004618	-3.740183	-0.762065
H	0.265821	-2.138627	-1.003094
H	-0.145529	-3.134496	0.398007
C	-1.400018	-1.533195	2.368381
C	-0.235837	-1.885616	3.082810
H	-1.881552	-2.285503	1.737239
H	-2.072277	-0.777378	2.790220
H	-0.083732	-1.492566	4.090821
H	0.189816	-2.878634	2.928200

^{4}TS9-10A-04
Geometry with 77 atoms:
Total energy: -3045.571346960

Cr	0.100186	-0.504426	1.111554
P	1.385559	0.661553	-0.754789
P	-1.787913	0.017466	-0.540331
C	-1.078208	0.905355	-2.019928
C	0.376586	0.512784	-2.305096
H	-1.723002	0.752479	-2.898924
H	-1.143375	1.975555	-1.767822
H	0.447831	-0.535832	-2.633785
H	0.805945	1.139691	-3.102379
C	3.108928	0.259807	-1.198300
C	3.430383	-0.550936	-2.299908
C	4.132720	0.678848	-0.328018
C	4.756664	-0.928154	-2.529079
H	2.654940	-0.899683	-2.984871
C	5.454966	0.297670	-0.562388
H	3.898223	1.311768	0.531980
C	5.769483	-0.507723	-1.662299
H	4.998310	-1.554775	-3.391051
H	6.243358	0.632666	0.115991
H	6.804716	-0.806024	-1.844186
C	1.365983	2.452186	-0.359907
C	1.695062	3.442000	-1.301400
C	0.975269	2.837716	0.934264
C	1.622520	4.791826	-0.951761
H	2.011766	3.160574	-2.309143
C	0.904705	4.189542	1.284367
H	0.730664	2.071642	1.679610
C	1.226009	5.166621	0.338248
H	1.879049	5.557595	-1.687732
H	0.602244	4.477807	2.293970
H	1.171824	6.224635	0.605905
C	-2.533387	-1.534455	-1.158533
C	-3.286768	-2.309810	-0.256680
C	-2.305635	-2.021918	-2.455112
C	-3.813463	-3.539912	-0.652183
H	-3.475058	-1.943933	0.755716
C	-2.828294	-3.259962	-2.843804
H	-1.721191	-1.448750	-3.177313
C	-3.582223	-4.019862	-1.946441
H	-4.404856	-4.127993	0.053769
H	-2.645356	-3.628719	-3.856017
H	-3.990280	-4.985668	-2.253811
C	-3.178938	1.099044	-0.033442
C	-4.514127	0.851883	-0.390122
C	-2.868642	2.240816	0.727833
C	-5.521235	1.733518	0.014823
H	-4.775102	-0.027422	-0.982224
C	-3.876756	3.122242	1.122489
H	-1.832630	2.452004	1.006654
C	-5.206474	2.866710	0.770200
H	-6.558175	1.532861	-0.265585

H	-3.623847	4.008105	1.710230
H	-5.997395	3.551642	1.085220
C	1.741366	-0.641404	2.629704
C	2.334242	-1.858267	3.340984
C	1.822090	-3.236357	2.894385
C	2.267343	-3.741610	1.517091
C	1.930829	-2.866230	0.299128
C	0.496452	-2.334964	0.230733
H	2.197455	-0.547794	1.627190
H	1.991301	0.290338	3.157466
H	3.435041	-1.829319	3.228817
H	2.152405	-1.755316	4.424763
H	2.149484	-3.978352	3.642268
H	0.719116	-3.245098	2.940238
H	1.806999	-4.734935	1.370019
H	3.358165	-3.914148	1.530389
H	2.654308	-2.035881	0.231683
H	2.135418	-3.468837	-0.605792
H	0.180188	-2.195691	-0.816837
H	-0.233101	-3.024929	0.693655
C	-1.404666	-0.673852	2.617211
C	-0.288925	-0.705884	3.474970
H	-1.930073	-1.610541	2.400786
H	-2.014270	0.234797	2.561144
H	-0.051102	0.184696	4.063117
H	-0.022229	-1.641887	3.964239

H	-3.701293	3.104443	2.906707
H	-5.675623	3.708159	1.508165
C	1.582147	-0.800194	2.772851
C	2.666985	-1.868156	2.905966
C	3.258231	-2.408421	1.591076
C	2.600232	-3.664696	1.009814
C	1.084713	-3.608931	0.785095
C	0.585530	-2.404058	-0.011246
H	1.923636	-0.033903	2.043474
H	1.468802	-0.246396	3.712536
H	3.486418	-1.410973	3.489831
H	2.308617	-2.704774	3.534405
H	3.252998	-1.604153	0.838296
H	4.323648	-2.640014	1.754474
H	2.824037	-4.525239	1.665348
H	3.091492	-3.884156	0.044775
H	0.791260	-4.533057	0.251072
H	0.560284	-3.681309	1.752718
H	1.307769	-2.136615	-0.802079
H	-0.377614	-2.635077	-0.493807
C	-1.400268	-1.601222	2.329966
C	-0.339836	-1.657093	3.262268
H	-1.674827	-2.502124	1.771513
H	-2.223784	-0.905212	2.522207
H	-0.399504	-1.006087	4.137419
H	0.169713	-2.603107	3.454449

H	-3.320138	3.693849	2.704933
H	-4.453489	5.105307	0.989513
C	1.206430	-2.358549	1.743328
C	0.441085	-2.918434	0.524040
C	-0.491440	-4.114027	0.781200
C	-1.898721	-3.765564	1.279212
C	-1.949935	-2.815248	2.485315
C	-1.814705	-1.329748	2.125725
H	2.248207	-2.158175	1.472893
H	1.177157	-3.097829	2.549054
H	-0.181141	-2.174698	-0.067415
H	1.207355	-3.179434	-0.223884
H	-0.581109	-4.682750	-0.159396
H	0.005859	-4.788784	1.499167
H	-2.407336	-4.712008	1.526765
H	-2.477614	-3.318578	0.450698
H	-2.917061	-2.968471	3.000622
H	-1.182901	-3.116569	3.223097
H	-2.684961	-1.047338	1.508451
H	-1.884095	-0.720280	3.044166
C	0.610079	0.391556	2.792287
C	1.036830	-0.919823	3.181585
H	-0.262129	0.813523	3.300573
H	1.383757	1.120858	2.530381
H	2.102620	-1.081041	3.364668
H	0.394619	-1.466821	3.877111

^{4}TS9-10A-05
Geometry with 77 atoms:
Total energy: -3045.571796370

Cr	0.097611	-0.720155	1.096585
P	1.372367	0.739960	-0.614929
P	-1.782725	-0.008999	-0.462447
C	-1.069027	0.881568	-1.945775
C	0.400933	0.514351	-2.186000
H	-1.683523	0.680383	-2.836419
H	-1.165151	1.956364	-1.726342
H	0.497898	-0.542826	-2.476661
H	0.837554	1.127367	-2.989970
C	3.109534	0.348368	-1.019413
C	3.446320	-0.591756	-2.009053
C	4.129330	0.895553	-0.217813
C	4.778387	-0.975891	-2.189970
H	2.678747	-1.032577	-2.647596
C	5.457467	0.509722	-0.405258
H	3.887248	1.630242	0.554343
C	5.784873	-0.429978	-1.388650
H	5.028658	-1.705187	-2.964174
H	6.240553	0.944183	0.220824
H	6.824523	-0.733880	-1.531965
C	1.320179	2.551855	-0.344211
C	1.979456	3.446558	-1.206265
C	0.552461	3.060586	0.715754
C	1.864488	4.823443	-1.008029
H	2.590348	3.067210	-2.029291
C	0.434413	4.440029	0.910138
H	0.033475	2.379803	1.394941
C	1.090925	5.321702	0.047819
H	2.380461	5.513043	-1.680560
H	-0.170391	4.823391	1.735283
H	1.002983	6.400432	0.198399
C	-2.720323	-1.430386	-1.134873
C	-3.770796	-1.978074	-0.376262
C	-2.340825	-2.057779	-2.333766
C	-4.434656	-3.124491	-0.817649
H	-4.081936	-1.502448	0.556703
C	-3.008833	-3.205748	-2.770298
H	-1.520683	-1.662920	-2.937296
C	-4.055305	-3.741389	-2.014553
H	-5.254730	-3.536047	-0.224296
H	-2.708192	-3.682579	-3.706390
H	-4.576393	-4.638199	-2.358056
C	-3.055439	1.143615	0.179220
C	-4.175207	1.483810	-0.600985
C	-2.895601	1.732752	1.444027
C	-5.110557	2.403184	-0.123059
H	-4.321643	1.022164	-1.580749
C	-3.833640	2.653916	1.920082
H	-2.040389	1.470292	2.071993
C	-4.940333	2.990498	1.136242
H	-5.978481	2.661211	-0.734757

^{4}TS9-10A-06
Geometry with 77 atoms:
Total energy: -3045.576289720

Cr	-0.071595	-0.678390	1.154994
P	1.773874	0.268911	-0.472273
P	-1.463332	0.489542	-0.587886
C	-0.412272	1.057204	-2.034019
C	0.928165	0.314210	-2.131522
H	-0.985151	0.951732	-2.967697
H	-0.239194	2.133046	-1.876543
H	0.778859	-0.730460	-2.446496
H	1.583081	0.793062	-2.876351
C	3.320689	-0.675895	-0.714043
C	3.563286	-1.475759	-1.843633
C	4.263405	-0.668850	0.333447
C	4.727020	-2.249002	-1.923235
H	2.857757	-1.499329	-2.676377
C	5.425164	-1.436749	0.245960
H	4.095420	-0.047174	1.217555
C	5.658484	-2.231563	-0.882432
H	4.907349	-2.862229	-2.809532
H	6.152268	-1.414600	1.061426
H	6.567586	-2.833799	-0.949701
C	2.284001	2.018509	-0.236364
C	3.513673	2.509128	-0.709518
C	1.380539	2.906437	0.376360
C	3.830240	3.862747	-0.569161
H	4.228153	1.834370	-1.186354
C	1.697249	4.261415	0.504059
H	0.421238	2.546158	0.754325
C	2.923771	4.740709	0.034958
H	4.789883	4.234025	-0.937229
H	0.983722	4.940569	0.976860
H	3.175117	5.798842	0.141434
C	-2.661246	-0.702945	-1.304346
C	-4.009171	-0.699282	-0.909338
C	-2.200233	-1.721895	-2.157592
C	-4.877886	-1.696216	-1.363555
H	-4.386396	0.082340	-0.246548
C	-3.072694	-2.713741	-2.610985
H	-1.156692	-1.751534	-2.477478
C	-4.413317	-2.705390	-2.211605
H	-5.924579	-1.681833	-1.050419
H	-2.703253	-3.496910	-3.277479
H	-5.094637	-3.483903	-2.562850
C	-2.433353	1.958616	-0.102144
C	-3.079679	2.753773	-1.065939
C	-2.524331	2.303333	1.255989
C	-3.800415	3.882015	-0.671262
H	-3.024900	2.491792	-2.125715
C	-3.251133	3.432622	1.646228
H	-2.031016	1.687150	2.010217
C	-3.886704	4.222222	0.684292
H	-4.299339	4.497612	-1.423671

^{4}TS9-10A-07
Geometry with 77 atoms:
Total energy: -3045.569890560

Cr	0.095625	-0.651222	1.030883
P	1.356171	0.800012	-0.709161
P	-1.830260	0.102396	-0.467751
C	-1.142741	1.124659	-1.872579
C	0.296134	0.731371	-2.234149
H	-1.812706	1.064102	-2.744428
H	-1.177355	2.167274	-1.518924
H	0.335867	-0.301387	-2.614925
H	0.704484	1.394554	-3.013138
C	3.028055	0.238483	-1.178368
C	3.279027	-0.542204	-2.319079
C	4.078124	0.492888	-0.274723
C	4.559431	-1.054613	-2.551762
H	2.485449	-0.757321	-3.036999
C	5.353653	-0.020953	-0.512815
H	3.899726	1.100980	0.616153
C	5.596540	-0.798132	-1.651008
H	4.745610	-1.655920	-3.444933
H	6.161832	0.187172	0.192509
H	6.594976	-1.201445	-1.835981
C	1.511531	2.589963	-0.355085
C	2.189639	3.456215	-1.231095
C	0.915546	3.112599	0.804142
C	2.259831	4.821710	-0.950387
H	2.672063	3.061041	-2.129258
C	0.984019	4.481273	1.082071
H	0.395068	2.448888	1.500012
C	1.655478	5.335656	0.203849
H	2.789587	5.489867	-1.633709
H	0.515595	4.878048	1.985931
H	1.713197	6.405300	0.419748
C	-2.708742	-1.309497	-1.230102
C	-3.575246	-2.064723	-0.417627
C	-2.468675	-1.726096	-2.549321
C	-4.198053	-3.206816	-0.922432
H	-3.774947	-1.751128	0.610005
C	-3.091718	-2.874961	-3.048473
H	-1.797853	-1.165295	-3.203048
C	-3.955281	-3.616457	-2.238641
H	-4.876259	-3.779839	-0.285487
H	-2.900822	-3.187847	-4.077888
H	-4.441647	-4.512273	-2.632014
C	-3.138698	1.174080	0.239335
C	-4.422757	1.254882	-0.326054
C	-2.825957	1.974095	1.351534
C	-5.373183	2.124153	0.215310
H	-4.684850	0.633301	-1.185327
C	-3.777053	2.845935	1.887444
H	-1.833725	1.920295	1.806857
C	-5.052759	2.920261	1.320155
H	-6.370302	2.179580	-0.228189

H	-3.523488	3.462208	2.753422
H	-5.799959	3.596919	1.741888
C	1.772211	-0.854424	2.387390
C	2.609743	-1.835514	3.193166
C	2.537956	-3.314497	2.764345
C	2.413100	-3.617835	1.258642
C	0.979729	-3.624777	0.673600
C	0.484201	-2.366986	-0.038840
H	2.190066	-0.850877	1.362049
H	1.861045	0.172741	2.784482
H	3.659564	-1.497519	3.106867
H	2.369766	-1.758792	4.268105
H	3.445496	-3.805918	3.151643
H	1.703917	-3.820442	3.281264
H	2.834854	-4.623564	1.102042
H	3.057962	-2.939150	0.670844
H	0.930447	-4.443420	-0.070275
H	0.263100	-3.925232	1.459849
H	1.204119	-2.075158	-0.825777
H	-0.482557	-2.574244	-0.527356
C	-1.353346	-1.298091	2.461601
C	-0.189961	-1.476007	3.228539
H	-1.825745	-2.172530	2.002379
H	-2.017377	-0.452380	2.670669
H	0.033981	-0.785305	4.046139
H	0.189510	-2.485920	3.375780

^{4}TS9-10A-08
Geometry with 77 atoms:
Total energy: -3045.575196300

Cr	0.077805	-0.284702	1.278761
P	1.567734	-0.278313	-0.687002
P	-1.707055	-0.117056	-0.650181
C	-0.737636	-0.041236	-2.238794
C	0.562947	-0.847642	-2.152052
H	-1.361235	-0.354172	-3.090207
H	-0.514994	1.026780	-2.392253
H	0.357577	-1.920294	-2.014548
H	1.157288	-0.742047	-3.072608
C	3.003380	-1.409057	-0.608976
C	2.797820	-2.798357	-0.690073
C	4.295651	-0.920035	-0.352414
C	3.871367	-3.678972	-0.539467
H	1.799067	-3.205216	-0.862773
C	5.364805	-1.806751	-0.197428
H	4.474415	0.154419	-0.276039
C	5.156821	-3.185551	-0.293655
H	3.700988	-4.755952	-0.611193
H	6.365927	-1.414966	-0.001800
H	5.994949	-3.876396	-0.174607
C	2.214370	1.345263	-1.247947
C	2.979986	1.454737	-2.423512
C	1.906648	2.506320	-0.521656
C	3.421162	2.704799	-2.860710
H	3.242048	0.560573	-2.994842
C	2.348047	3.758147	-0.962055
H	1.332531	2.436762	0.403078
C	3.104243	3.858042	-2.132266
H	4.017350	2.780465	-3.773261
H	2.104119	4.653826	-0.385560
H	3.452321	4.834620	-2.477497
C	-2.782629	-1.596196	-0.765126
C	-3.727511	-1.818752	0.256312
C	-2.632854	-2.566498	-1.770208
C	-4.512077	-2.973189	0.260547
H	-3.865112	-1.079129	1.048796
C	-3.413078	-3.727618	-1.755959
H	-1.912156	-2.432746	-2.578699
C	-4.353760	-3.933875	-0.744415
H	-5.248981	-3.123981	1.053185
H	-3.285641	-4.471449	-2.546332
H	-4.963828	-4.840211	-0.738650
C	-2.800569	1.353597	-0.734127
C	-4.181027	1.296016	-0.981540
C	-2.191374	2.605472	-0.523733
C	-4.937018	2.472511	-1.012297
H	-4.671962	0.336208	-1.153059
C	-2.948033	3.777582	-0.566150
H	-1.115070	2.668062	-0.339000
C	-4.325441	3.712050	-0.805097
H	-6.011109	2.417697	-1.206113

H	-2.462684	4.743952	-0.408699
H	-4.920621	4.628044	-0.830953
C	-1.485835	-0.054643	2.824787
C	-0.890812	1.349749	2.676706
C	0.034651	1.863869	3.801205
C	1.409761	2.320609	3.295514
C	2.366310	1.173384	2.873837
C	1.719453	-0.182662	2.554329
H	-2.480140	-0.109787	2.369092
H	-1.560512	-0.303595	3.887450
H	-0.360375	1.531255	1.685733
H	-1.737268	2.037118	2.511526
H	-0.466030	2.708433	4.300085
H	0.157515	1.085513	4.570549
H	1.894767	2.930047	4.074244
H	1.245580	3.015107	2.450524
H	2.970126	1.512451	2.014659
H	3.095948	1.020955	3.691464
H	2.490496	-0.871814	2.170510
H	1.343042	-0.641131	3.487322
C	-0.074507	-2.354077	1.396925
C	-0.894716	-2.028887	2.519861
H	0.932520	-2.734255	1.593751
H	-0.570232	-2.773751	0.514067
H	-1.955719	-2.288289	2.475916
H	-0.453682	-2.148626	3.512033

^{4}TS9-10A-09
Geometry with 77 atoms:
Total energy: -3045.577760610

Cr	0.126428	-0.248410	1.290889
P	1.563367	-0.259655	-0.725725
P	-1.726437	-0.102185	-0.626159
C	-0.779993	-0.020509	-2.228437
C	0.527056	-0.820123	-2.171394
H	-1.417312	-0.334039	-3.069733
H	-0.566053	1.049870	-2.380319
H	0.332974	-1.895310	-2.039045
H	1.102901	-0.703397	-3.102460
C	2.988035	-1.404906	-0.668992
C	2.765303	-2.792368	-0.737685
C	4.288919	-0.929448	-0.430793
C	3.830397	-3.684427	-0.594800
H	1.759701	-3.189187	-0.893560
C	5.349651	-1.827612	-0.284112
H	4.480753	0.143168	-0.360505
C	5.124577	-3.204458	-0.368933
H	3.646540	-4.759823	-0.656371
H	6.357601	-1.446379	-0.103277
H	5.956087	-3.904262	-0.255901
C	2.208532	1.360694	-1.291660
C	2.981248	1.470588	-2.462292
C	1.885785	2.521668	-0.572027
C	3.416955	2.722378	-2.900042
H	3.252695	0.575982	-3.028458
C	2.320908	3.775112	-1.013345
H	1.301026	2.447844	0.346467
C	3.086296	3.875643	-2.177687
H	4.019277	2.799503	-3.808438
H	2.065266	4.671440	-0.443070
H	3.430239	4.853419	-2.523671
C	-2.759693	-1.613869	-0.711525
C	-3.687606	-1.842259	0.323711
C	-2.603487	-2.592025	-1.707636
C	-4.446041	-3.013451	0.353485
H	-3.834649	-1.092693	1.105048
C	-3.357837	-3.769842	-1.668354
H	-1.899537	-2.450237	-2.529398
C	-4.279162	-3.983995	-0.640839
H	-5.170094	-3.169464	1.156903
H	-3.225983	-4.520122	-2.451888
H	-4.868844	-4.903390	-0.615197
C	-2.881180	1.319098	-0.732873
C	-4.220021	1.199880	-1.139292
C	-2.373333	2.589151	-0.401669
C	-5.034621	2.334056	-1.209910
H	-4.631332	0.222696	-1.400526
C	-3.187957	3.720433	-0.482548
H	-1.332515	2.699665	-0.085437
C	-4.522384	3.593241	-0.882814
H	-6.075415	2.232121	-1.527020

H	-2.781752	4.702372	-0.227721
H	-5.163294	4.476479	-0.939030
C	-1.419660	0.003719	2.900906
C	-0.821562	1.410228	2.788669
C	0.157467	1.867043	3.891447
C	1.507046	2.350221	3.342067
C	2.449492	1.229253	2.822325
C	1.809519	-0.134243	2.520090
H	-2.409636	-0.042847	2.432858
H	-1.504773	-0.269247	3.957021
H	-0.335344	1.627755	1.784675
H	-1.672384	2.106949	2.697102
H	-0.315616	2.685110	4.456959
H	0.317785	1.050708	4.613088
H	2.026952	2.923022	4.126142
H	1.303504	3.085039	2.541042
H	2.981791	1.597509	1.928839
H	3.240742	1.072702	3.579571
H	2.576273	-0.811571	2.107422
H	1.469161	-0.602335	3.461888
C	-0.034386	-2.326556	1.452593
C	-0.820977	-2.005298	2.597795
H	0.982598	-2.697180	1.615194
H	-0.555008	-2.745035	0.583495
H	-1.885083	-2.254851	2.584576
H	-0.351186	-2.104662	3.579085

^{4}TS9-10A-10
Geometry with 77 atoms:
Total energy: -3045.570506900

Cr	0.007158	-0.907747	-0.993209
P	-1.704892	0.453555	0.547702
P	1.564327	0.435054	0.534254
C	0.599216	1.229936	1.934326
C	-0.775788	0.586961	2.158062
H	1.199379	1.199774	2.856073
H	0.482068	2.289331	1.659807
H	-0.674716	-0.439563	2.547414
H	-1.360690	1.166024	2.890191
C	-3.325056	-0.287923	0.953988
C	-3.600160	-0.913074	2.180727
C	-4.306059	-0.303744	-0.057198
C	-4.833292	-1.541032	2.390336
H	-2.864891	-0.914002	2.987482
C	-5.536867	-0.923833	0.159353
H	-4.110511	0.184238	-1.016612
C	-5.801764	-1.548359	1.384020
H	-5.037008	-2.021977	3.350243
H	-6.292337	-0.921214	-0.630234
H	-6.764166	-2.037408	1.552851
C	-2.063384	2.209176	0.133568
C	-3.211666	2.869291	0.606659
C	-1.128210	2.929253	-0.631952
C	-3.414567	4.220986	0.317508
H	-3.952519	2.329649	1.200651
C	-1.329572	4.284125	-0.909475
H	-0.228902	2.439095	-1.008280
C	-2.475118	4.931189	-0.438035
H	-4.311341	4.723587	0.688308
H	-0.589157	4.830130	-1.499100
H	-2.637842	5.988826	-0.659565
C	2.785187	-0.655639	1.365208
C	4.063695	-0.832594	0.809408
C	2.416253	-1.413638	2.490150
C	4.954071	-1.751904	1.370244
H	4.372339	-0.247498	-0.059728
C	3.310843	-2.330104	3.048534
H	1.428368	-1.300030	2.942607
C	4.579880	-2.504508	2.487730
H	5.946862	-1.877868	0.931468
H	3.014324	-2.910306	3.925791
H	5.277940	-3.223144	2.923700
C	2.557827	1.805642	-0.158675
C	3.300543	2.647458	0.689034
C	2.570224	2.031877	-1.543442
C	4.033188	3.707736	0.153847
H	3.311561	2.472339	1.768003
C	3.307809	3.094788	-2.075763
H	2.004400	1.376296	-2.207184
C	4.035818	3.933680	-1.228241
H	4.607409	4.359737	0.816580

H	3.313131	3.265232	-3.154996
H	4.611301	4.764620	-1.643577
C	-1.518236	-2.435573	-1.227871
C	-1.449731	-3.811249	-1.874090
C	-0.075607	-4.340060	-2.306246
C	1.027312	-4.417797	-1.239932
C	1.569778	-3.089425	-0.664005
C	1.665153	-1.926266	-1.653797
H	-1.105018	-2.484356	-0.190681
H	-2.557645	-2.108875	-1.108248
H	-1.895315	-4.526398	-1.155034
H	-2.123336	-3.828026	-2.748737
H	-0.226456	-5.356797	-2.705886
H	0.289921	-3.749237	-3.162328
H	1.880584	-4.943909	-1.701506
H	0.691253	-5.063216	-0.408960
H	0.949706	-2.791226	0.220585
H	2.546560	-3.279480	-0.187955
H	2.605854	-1.364430	-1.556919
H	1.570552	-2.233970	-2.705337
C	-0.389050	0.043645	-2.862818
C	-1.211234	-1.080339	-3.017419
H	0.582322	0.062284	-3.364905
H	-0.850601	1.013890	-2.654616
H	-2.296743	-0.968776	-2.979476
H	-0.858564	-1.928654	-3.606673

H	-3.206473	3.465530	3.010231
H	-4.327658	5.006248	1.400039
C	1.471793	-2.353531	1.612449
C	0.899831	-3.641473	2.201697
C	0.058773	-4.462632	1.204324
C	-1.039366	-3.710386	0.443975
C	-2.101852	-2.995306	1.294983
C	-1.608620	-1.754356	2.057949
H	1.378579	-2.326720	0.501182
H	2.546596	-2.243657	1.790083
H	1.729084	-4.276722	2.557423
H	0.300466	-3.426123	3.101097
H	0.740236	-4.919133	0.464513
H	-0.403925	-5.302350	1.750937
H	-1.538272	-4.424689	-0.232562
H	-0.579926	-2.965792	-0.243470
H	-2.916319	-2.698615	0.617796
H	-2.547360	-3.731175	1.991783
H	-2.435903	-1.038332	2.208567
H	-1.239398	-2.015119	3.064520
C	0.413496	0.365702	2.899476
C	1.336355	-0.656872	3.135890
H	-0.531289	0.369287	3.450178
H	0.773694	1.332451	2.535064
H	2.399553	-0.466261	2.974406
H	1.114486	-1.447648	3.856358

H	-3.970466	4.211285	1.670295
H	-6.051349	3.987104	0.314023
C	1.294001	-1.369525	2.492730
C	0.630230	-2.407879	1.563374
C	-0.149947	-3.531872	2.263039
C	-1.585241	-3.204783	2.696222
C	-1.779789	-1.874022	3.438820
C	-1.823077	-0.630430	2.541153
H	2.310943	-1.150318	2.152836
H	1.337561	-1.780104	3.505613
H	-0.044625	-1.999889	0.747201
H	1.442150	-2.828253	0.948446
H	-0.177342	-4.401184	1.585229
H	0.438593	-3.850808	3.140436
H	-1.936787	-4.035492	3.330299
H	-2.242911	-3.213731	1.809145
H	-2.733111	-1.936599	3.997247
H	-1.001418	-1.773110	4.217367
H	-2.694289	-0.705050	1.866287
H	-2.014208	0.264996	3.157389
C	0.344876	1.499872	2.617140
C	0.925536	0.456878	3.401184
H	-0.595826	1.937545	2.963569
H	1.032588	2.194392	2.129536
H	2.002086	0.488993	3.587718
H	0.346509	0.078865	4.247318

^{4}TS9-10A-11
Geometry with 77 atoms:
Total energy: -3045.569853210

Cr	0.010780	-0.813797	1.158750
P	1.734935	0.358113	-0.522314
P	-1.560085	0.365029	-0.506876
C	-0.575790	1.005661	-1.972933
C	0.789956	0.325739	-2.127810
H	-1.173311	0.888172	-2.889143
H	-0.445330	2.085740	-1.806567
H	0.670639	-0.736031	-2.401992
H	1.374865	0.812392	-2.924353
C	3.314576	-0.499248	-0.856062
C	3.586536	-1.179564	-2.054361
C	4.267935	-0.532384	0.180359
C	4.788616	-1.879228	-2.209814
H	2.874035	-1.169043	-2.881123
C	5.469187	-1.222609	0.017167
H	4.074415	-0.001981	1.117138
C	5.730153	-1.902513	-1.178499
H	4.989872	-2.403346	-3.147384
H	6.203915	-1.232875	0.825994
H	6.668645	-2.447427	-1.305409
C	2.161039	2.132062	-0.311135
C	3.366513	2.680962	-0.781649
C	1.222485	2.972691	0.315422
C	3.624030	4.045378	-0.624307
H	4.108116	2.044531	-1.269342
C	1.479836	4.338331	0.460641
H	0.279063	2.567038	0.686255
C	2.683503	4.875702	-0.005109
H	4.565463	4.462552	-0.990301
H	0.738711	4.979387	0.944091
H	2.890601	5.941850	0.115545
C	-2.847487	-0.707901	-1.250669
C	-4.168219	-0.683805	-0.773119
C	-2.489752	-1.638517	-2.241475
C	-5.114398	-1.577147	-1.282653
H	-4.463085	0.031769	-0.002812
C	-3.440014	-2.527700	-2.748590
H	-1.466655	-1.679751	-2.624686
C	-4.753287	-2.501140	-2.267764
H	-6.139952	-1.548832	-0.906732
H	-3.153039	-3.244736	-3.521476
H	-5.495180	-3.198994	-2.663208
C	-2.464107	1.840219	0.096275
C	-3.107396	2.706706	-0.806728
C	-2.508213	2.120310	1.470744
C	-3.771689	3.840480	-0.336346
H	-3.096471	2.496521	-1.879202
C	-3.177551	3.256142	1.938224
H	-2.020289	1.450553	2.179057
C	-3.806103	4.117702	1.035849
H	-4.267306	4.510459	-1.043071

^{4}TS9-10A-12
Geometry with 77 atoms:
Total energy: -3045.574473370

Cr	-0.143696	-0.116207	1.390110
P	1.732667	0.446793	-0.522479
P	-1.583717	0.528566	-0.596793
C	-0.536427	1.475536	-1.807468
C	0.772861	0.732668	-2.099878
H	-1.103013	1.675268	-2.730073
H	-0.351419	2.457657	-1.344411
H	0.554318	-0.245038	-2.551977
H	1.400061	1.291762	-2.810666
C	2.866153	-0.959721	-0.836143
C	2.621819	-1.925078	-1.828113
C	3.937430	-1.165242	0.056978
C	3.430308	-3.062196	-1.926166
H	1.799780	-1.807276	-2.536321
C	4.744804	-2.299270	-0.047190
H	4.155057	-0.427402	0.833496
C	4.491253	-3.254229	-1.037598
H	3.228044	-3.799970	-2.706446
H	5.575132	-2.436915	0.649756
H	5.121120	-4.143381	-1.117329
C	2.781363	1.958943	-0.453271
C	4.116293	1.988354	-0.893464
C	2.185001	3.155816	-0.013547
C	4.838406	3.184944	-0.876138
H	4.600172	1.081264	-1.259374
C	2.907364	4.351922	-0.008436
H	1.145876	3.163080	0.320583
C	4.238890	4.367743	-0.432848
H	5.875969	3.191641	-1.219109
H	2.427342	5.272114	0.333458
H	4.807646	5.300633	-0.421416
C	-2.183284	-0.925633	-1.552754
C	-2.771399	-1.991165	-0.846903
C	-2.079913	-1.017344	-2.952347
C	-3.240327	-3.120444	-1.521021
H	-2.873439	-1.937798	0.236917
C	-2.544323	-2.152623	-3.624072
H	-1.641605	-0.208236	-3.538424
C	-3.123586	-3.206383	-2.911848
H	-3.697944	-3.935698	-0.955356
H	-2.455044	-2.209218	-4.711693
H	-3.485696	-4.091690	-3.440116
C	-3.044152	1.595244	-0.325315
C	-4.218857	1.468772	-1.084337
C	-2.963442	2.582827	0.671927
C	-5.295145	2.329353	-0.851599
H	-4.298634	0.697431	-1.853793
C	-4.039309	3.444952	0.894297
H	-2.059890	2.673363	1.280296
C	-5.206572	3.317830	0.133801
H	-6.208281	2.225446	-1.442756

^{4}TS9-10A-13
Geometry with 77 atoms:
Total energy: -3045.570498070

Cr	0.002418	-0.769952	1.223562
P	1.774512	0.233054	-0.474867
P	-1.507369	0.366310	-0.488289
C	-0.487043	0.920562	-1.967628
C	0.849935	0.180077	-2.090142
H	-1.083968	0.799517	-2.883649
H	-0.312903	1.999034	-1.833981
H	0.687720	-0.882666	-2.334389
H	1.463159	0.618399	-2.893353
C	3.327530	-0.692361	-0.753324
C	3.556398	-1.489559	-1.887280
C	4.301521	-0.656970	0.264629
C	4.735836	-2.234721	-1.998983
H	2.827779	-1.534143	-2.698786
C	5.478859	-1.396182	0.145268
H	4.143988	-0.035230	1.150794
C	5.697289	-2.190201	-0.986694
H	4.904334	-2.847226	-2.888108
H	6.229176	-1.353235	0.938546
H	6.618325	-2.770583	-1.079240
C	2.271241	1.998956	-0.343831
C	3.494365	2.471581	-0.851729
C	1.371012	2.913282	0.234297
C	3.807215	3.831368	-0.778555
H	4.207765	1.779156	-1.303559
C	1.684197	4.273801	0.295383
H	0.415235	2.571039	0.635047
C	2.904355	4.734457	-0.207342
H	4.761850	4.187272	-1.173839
H	0.972230	4.971681	0.742548
H	3.153341	5.797071	-0.152953
C	-2.817206	-0.689682	-1.224978
C	-4.152408	-0.582773	-0.802538
C	-2.474117	-1.665211	-2.177453
C	-5.125844	-1.437509	-1.326862
H	-4.437114	0.167890	-0.062433
C	-3.451179	-2.515962	-2.699936
H	-1.441735	-1.769816	-2.522092
C	-4.778503	-2.405889	-2.273426
H	-6.161773	-1.344360	-0.992050
H	-3.173887	-3.268342	-3.442184
H	-5.541731	-3.073068	-2.681042
C	-2.380632	1.889256	0.038631
C	-2.964005	2.747944	-0.911525
C	-2.469198	2.208827	1.402291
C	-3.614491	3.911596	-0.498227
H	-2.917953	2.509131	-1.977053
C	-3.125777	3.374041	1.812260
H	-2.025068	1.547539	2.146268
C	-3.695542	4.226705	0.863720
H	-4.063612	4.574597	-1.241704

H	-3.190170	3.613366	2.876462
H	-4.207346	5.137675	1.183719
C	1.490134	-2.256563	1.956098
C	0.728783	-3.003373	0.861256
C	-0.272876	-4.097397	1.292641
C	-1.704445	-3.823897	0.815623
C	-2.462590	-2.755098	1.629388
C	-1.641151	-1.587885	2.206256
H	2.501658	-2.000837	1.627106
H	1.541144	-2.882526	2.851621
H	0.177639	-2.332674	0.124358
H	1.488320	-3.404713	0.169146
H	0.072459	-5.059457	0.882970
H	-0.257119	-4.206236	2.389564
H	-2.283537	-4.761418	0.833317
H	-1.664221	-3.525998	-0.247669
H	-3.276723	-2.367687	0.999513
H	-2.965109	-3.265867	2.473072
H	-2.321048	-0.756209	2.460441
H	-1.180605	-1.899794	3.161190
C	0.460588	0.486173	2.826665
C	1.225651	-0.638617	3.249104
H	-0.467653	0.694692	3.366961
H	0.999832	1.366902	2.464634
H	2.315023	-0.551188	3.273208
H	0.819700	-1.245955	4.061115

H	-3.128261	3.672114	2.846243
H	-4.204428	5.154580	1.153099
C	1.446058	-2.294922	1.953581
C	0.639778	-3.050947	0.894415
C	-0.410282	-4.076177	1.379738
C	-1.836571	-3.754677	0.912793
C	-2.545118	-2.637110	1.707026
C	-1.672414	-1.492669	2.250925
H	2.450585	-2.058251	1.589010
H	1.518316	-2.909070	2.856060
H	0.125840	-2.388208	0.126901
H	1.380340	-3.523293	0.226436
H	-0.119349	-5.068536	1.001156
H	-0.381674	-4.146675	2.479598
H	-2.452057	-4.667651	0.960426
H	-1.796438	-3.485609	-0.157861
H	-3.347349	-2.230993	1.073383
H	-3.061799	-3.106987	2.565819
H	-2.317352	-0.634086	2.507397
H	-1.205006	-1.810463	3.200623
C	0.517582	0.492322	2.833857
C	1.245890	-0.657097	3.257819
H	-0.397151	0.738916	3.381518
H	1.086496	1.351481	2.464492
H	2.338206	-0.612100	3.268256
H	0.824894	-1.249809	4.073060

H	3.181908	2.985962	-3.339229
H	4.843793	4.341079	-2.065293
C	-1.283131	-2.628465	-0.734891
C	-1.567958	-3.966058	-1.392380
C	-0.561793	-4.537590	-2.406506
C	0.938332	-4.405186	-2.095331
C	1.618635	-3.084163	-2.519033
C	1.699997	-1.974899	-1.468233
H	-0.438958	-2.751435	0.001030
H	-2.170969	-2.278193	-0.190264
H	-1.683603	-4.693253	-0.565136
H	-2.563695	-3.922130	-1.866651
H	-0.808449	-5.605971	-2.521570
H	-0.742712	-4.101583	-3.404854
H	1.446622	-5.224715	-2.628887
H	1.126685	-4.596417	-1.022345
H	2.652797	-3.331811	-2.825482
H	1.137295	-2.709751	-3.442471
H	2.150446	-2.379763	-0.539809
H	2.392043	-1.186205	-1.819835
C	-0.569662	-0.204308	-2.711194
C	-1.432358	-1.297754	-2.620066
H	0.318765	-0.279077	-3.345696
H	-0.949230	0.802641	-2.516158
H	-2.477949	-1.155929	-2.335227
H	-1.226634	-2.192925	-3.204107

^{4}TS9-10A-14
Geometry with 77 atoms:
Total energy: -3045.573506640

Cr	-0.013789	-0.747576	1.230652
P	1.784666	0.222925	-0.484179
P	-1.499420	0.381962	-0.501568
C	-0.470028	0.944833	-1.971218
C	0.860772	0.194168	-2.100291
H	-1.066408	0.839140	-2.889587
H	-0.287957	2.020177	-1.823704
H	0.688584	-0.864683	-2.354074
H	1.477897	0.634492	-2.899378
C	3.325196	-0.721991	-0.764542
C	3.550393	-1.507872	-1.907078
C	4.291561	-0.715257	0.261262
C	4.719219	-2.269327	-2.019934
H	2.827128	-1.530824	-2.724258
C	5.458600	-1.470437	0.140642
H	4.137040	-0.103194	1.154744
C	5.673626	-2.252673	-1.000177
H	4.885060	-2.872693	-2.915798
H	6.203529	-1.449198	0.939857
H	6.586473	-2.845691	-1.093691
C	2.303570	1.980913	-0.339313
C	3.536015	2.440897	-0.835822
C	1.411113	2.902988	0.238707
C	3.865555	3.796191	-0.752319
H	4.243352	1.741944	-1.287211
C	1.741005	4.259008	0.310046
H	0.448725	2.570098	0.631758
C	2.970267	4.707202	-0.181842
H	4.827225	4.142403	-1.139081
H	1.035031	4.963227	0.756796
H	3.232200	5.766255	-0.119418
C	-2.790497	-0.686090	-1.253489
C	-4.136859	-0.576621	-0.869257
C	-2.419667	-1.674893	-2.181872
C	-5.093927	-1.441017	-1.407940
H	-4.443244	0.183399	-0.147778
C	-3.380260	-2.534984	-2.719103
H	-1.377826	-1.782953	-2.495067
C	-4.719102	-2.421677	-2.331003
H	-6.138754	-1.345717	-1.102675
H	-3.081002	-3.297685	-3.442001
H	-5.469619	-3.096419	-2.749615
C	-2.380590	1.900808	0.020842
C	-2.994517	2.737345	-0.929774
C	-2.434732	2.245362	1.380306
C	-3.644567	3.902853	-0.521183
H	-2.971261	2.478434	-1.991401
C	-3.090036	3.412950	1.785450
H	-1.964874	1.601879	2.124396
C	-3.692783	4.242310	0.836543
H	-4.118356	4.548457	-1.264652

^{4}TS9-10A-15
Geometry with 77 atoms:
Total energy: -3045.568112850

Cr	0.028006	-0.973541	-0.793345
P	-1.670177	0.585032	0.583941
P	1.602852	0.470284	0.633127
C	0.641785	1.500227	1.868817
C	-0.751580	0.931059	2.169079
H	1.230813	1.610084	2.792237
H	0.556236	2.503818	1.424342
H	-0.679281	-0.026564	2.709907
H	-1.328013	1.627105	2.798838
C	-3.280145	-0.134474	1.066100
C	-3.576622	-0.570970	2.367499
C	-4.225596	-0.344167	0.042732
C	-4.795068	-1.204367	2.637406
H	-2.869219	-0.419651	3.184794
C	-5.441928	-0.969715	0.317960
H	-4.015743	-0.001298	-0.974655
C	-5.727869	-1.405348	1.617291
H	-5.015239	-1.537353	3.654635
H	-6.169423	-1.118309	-0.483722
H	-6.678238	-1.899419	1.833065
C	-2.056043	2.272037	-0.038320
C	-3.247138	2.939553	0.297777
C	-1.100508	2.935896	-0.829413
C	-3.472315	4.244016	-0.149260
H	-4.003746	2.441764	0.908187
C	-1.325340	4.244385	-1.265646
H	-0.169301	2.438435	-1.106579
C	-2.513029	4.899646	-0.928409
H	-4.402449	4.752519	0.116444
H	-0.570184	4.747924	-1.874072
H	-2.692847	5.920567	-1.273912
C	2.733294	-0.566777	1.636902
C	3.977657	-0.950863	1.105538
C	2.330612	-1.083294	2.881233
C	4.806359	-1.823636	1.814141
H	4.305365	-0.562112	0.139065
C	3.163716	-1.958142	3.584626
H	1.369304	-0.807929	3.321040
C	4.401967	-2.330319	3.053366
H	5.774409	-2.107980	1.394549
H	2.843063	-2.347310	4.554129
H	5.052416	-3.013101	3.605257
C	2.679556	1.678127	-0.220794
C	3.623749	2.439050	0.491761
C	2.528683	1.878512	-1.602279
C	4.396178	3.392950	-0.172771
H	3.762721	2.279665	1.564197
C	3.304131	2.836159	-2.263844
H	1.805045	1.283040	-2.162469
C	4.235899	3.593748	-1.549419
H	5.129088	3.981613	0.384358

^{4}TS9-10A-16
Geometry with 77 atoms:
Total energy: -3045.572712970

Cr	-0.068289	-0.911938	1.017268
P	1.766580	0.332404	-0.510388
P	-1.498332	0.446128	-0.609272
C	-0.454869	1.196398	-1.973983
C	0.898080	0.496059	-2.150196
H	-1.026778	1.187467	-2.914002
H	-0.304291	2.250969	-1.698061
H	0.766592	-0.526488	-2.540438
H	1.530729	1.047562	-2.863475
C	3.362811	-0.487133	-0.867630
C	3.653012	-1.106822	-2.094369
C	4.307345	-0.562972	0.175687
C	4.864035	-1.785186	-2.272650
H	2.947315	-1.063095	-2.925996
C	5.517057	-1.232882	-0.009936
H	4.102929	-0.080647	1.136128
C	5.796862	-1.849435	-1.235022
H	5.079584	-2.259827	-3.233111
H	6.244354	-1.274495	0.804596
H	6.742878	-2.376553	-1.380029
C	2.198391	2.075189	-0.103959
C	3.407016	2.665665	-0.514294
C	1.258894	2.858514	0.591603
C	3.666153	4.008986	-0.230031
H	4.152381	2.079607	-1.056083
C	1.517167	4.204617	0.863723
H	0.312397	2.425733	0.918386
C	2.723570	4.781254	0.457161
H	4.610362	4.455756	-0.551255
H	0.772495	4.799029	1.398714
H	2.930686	5.831700	0.675780
C	-2.714288	-0.613981	-1.486775
C	-4.023232	-0.744993	-0.991428
C	-2.319552	-1.387939	-2.592459
C	-4.920244	-1.627642	-1.598340
H	-4.348151	-0.153426	-0.132915
C	-3.220795	-2.269870	-3.195151
H	-1.308816	-1.309283	-2.999555
C	-4.522183	-2.392679	-2.698957
H	-5.937071	-1.715914	-1.208098
H	-2.904719	-2.860153	-4.058820
H	-5.226128	-3.081938	-3.171369
C	-2.474710	1.856596	0.028278
C	-3.223988	2.659336	-0.851055
C	-2.458855	2.159929	1.398553
C	-3.937897	3.754252	-0.362134
H	-3.254770	2.426450	-1.918591
C	-3.177588	3.257378	1.884354
H	-1.884687	1.539657	2.087964
C	-3.914737	4.054833	1.005420
H	-4.517510	4.375038	-1.049673

H	-3.161656	3.485936	2.952697
H	-4.476548	4.911985	1.384705
C	1.383141	-2.524187	1.464315
C	0.461726	-3.217396	0.468776
C	-0.506744	-4.267572	1.058300
C	-0.963085	-4.039057	2.508352
C	-1.857801	-2.802879	2.783307
C	-1.862403	-1.707925	1.712974
H	2.311334	-2.170666	1.002954
H	1.632062	-3.202196	2.283369
H	-0.119794	-2.498641	-0.189017
H	1.098257	-3.674499	-0.309766
H	-1.381046	-4.361017	0.393412
H	0.007927	-5.241986	1.020533
H	-0.068571	-4.002403	3.150832
H	-1.497564	-4.946994	2.830701
H	-2.899661	-3.151324	2.916693
H	-1.579812	-2.371452	3.760541
H	-2.343100	-2.099209	0.798588
H	-2.492466	-0.865947	2.051969
C	0.384935	0.083442	2.810588
C	1.122596	-1.099538	3.061757
H	-0.566129	0.214549	3.335683
H	0.937437	1.001305	2.586063
H	2.214719	-1.049030	3.079151
H	0.701124	-1.841181	3.742588

H	-3.216223	3.485404	2.920558
H	-4.465099	4.945894	1.330376
C	1.358160	-2.516810	1.481375
C	0.443675	-3.207140	0.477040
C	-0.537343	-4.251060	1.056847
C	-1.005960	-4.020096	2.502560
C	-1.896544	-2.778961	2.769018
C	-1.886129	-1.684863	1.697920
H	2.293567	-2.169900	1.029542
H	1.594513	-3.194829	2.304139
H	-0.126887	-2.486863	-0.188687
H	1.086469	-3.668876	-0.293587
H	-1.405817	-4.337852	0.383450
H	-0.029130	-5.229009	1.023428
H	-0.117364	-3.988245	3.153440
H	-1.548432	-4.925100	2.819785
H	-2.941357	-3.121813	2.893289
H	-1.624833	-2.348637	3.748556
H	-2.361480	-2.074516	0.779945
H	-2.516403	-0.840277	2.030308
C	0.363882	0.100450	2.810652
C	1.089991	-1.087361	3.073195
H	-0.591002	0.240988	3.326318
H	0.925485	1.013216	2.587794
H	2.182214	-1.045017	3.102507
H	0.655564	-1.824063	3.751287

H	-3.548969	3.471694	2.881252
H	-5.108845	4.549869	1.261691
C	1.751048	-2.064607	1.732873
C	1.536809	-3.452742	2.349970
C	0.955390	-4.499967	1.383843
C	-0.554181	-4.450411	1.107036
C	-1.142480	-3.098068	0.670796
C	-1.359120	-2.078170	1.785724
H	1.689964	-2.127193	0.622179
H	2.763025	-1.687895	1.913786
H	2.515611	-3.822921	2.698856
H	0.910486	-3.399050	3.257573
H	1.504532	-4.428575	0.426519
H	1.185927	-5.503254	1.779611
H	-1.103921	-4.779440	2.006003
H	-0.772936	-5.200164	0.327706
H	-0.475883	-2.669414	-0.136169
H	-2.080897	-3.262158	0.119542
H	-2.372752	-1.651466	1.794505
H	-1.129880	-2.464986	2.789443
C	0.066305	0.333140	2.929984
C	1.125121	-0.531996	3.238832
H	-0.917572	0.149283	3.369642
H	0.301339	1.368984	2.667518
H	2.144140	-0.140072	3.229785
H	0.965404	-1.374704	3.915202

^{4}TS9-10A-17
Geometry with 77 atoms:
Total energy: -3045.572732220

Cr	-0.080362	-0.897613	1.017615
P	1.764267	0.329371	-0.509852
P	-1.492684	0.457720	-0.618173
C	-0.448457	1.187154	-1.995310
C	0.909135	0.492231	-2.156695
H	-1.018023	1.154172	-2.936105
H	-0.304494	2.247733	-1.738810
H	0.785007	-0.527889	-2.554911
H	1.546816	1.048246	-2.861979
C	3.360945	-0.495191	-0.854423
C	3.660222	-1.114283	-2.079318
C	4.296364	-0.574600	0.196823
C	4.870702	-1.796151	-2.247750
H	2.962186	-1.067611	-2.917261
C	5.505584	-1.248067	0.021083
H	4.085510	-0.092104	1.155778
C	5.794159	-1.864444	-1.202057
H	5.093190	-2.270380	-3.206828
H	6.225673	-1.292623	0.841836
H	6.739726	-2.394432	-1.339280
C	2.198572	2.072047	-0.104923
C	3.411570	2.657140	-0.510126
C	1.258885	2.859972	0.585191
C	3.674862	3.999743	-0.226411
H	4.157390	2.067161	-1.047052
C	1.521547	4.205356	0.856884
H	0.309161	2.431645	0.908836
C	2.732177	4.776635	0.455381
H	4.622541	4.442130	-0.543465
H	0.776992	4.803458	1.387896
H	2.942589	5.826439	0.673935
C	-2.697345	-0.626865	-1.480050
C	-4.047240	-0.658743	-1.093512
C	-2.241693	-1.530446	-2.457360
C	-4.925903	-1.570979	-1.684996
H	-4.418830	0.029206	-0.331323
C	-3.124231	-2.439356	-3.045721
H	-1.194499	-1.533124	-2.769304
C	-4.468643	-2.462049	-2.660063
H	-5.975075	-1.583430	-1.379944
H	-2.759961	-3.131832	-3.808564
H	-5.158564	-3.173783	-3.119631
C	-2.467544	1.875818	0.000249
C	-3.179215	2.698594	-0.891849
C	-2.487446	2.165248	1.373622
C	-3.892101	3.798382	-0.412216
H	-3.181562	2.478470	-1.962436
C	-3.204929	3.267472	1.849945
H	-1.941170	1.530588	2.072616
C	-3.904981	4.084393	0.958516
H	-4.441819	4.434789	-1.109945

^{4}TS9-10A-18
Geometry with 77 atoms:
Total energy: -3045.569356880

Cr	0.075681	-0.803043	1.123205
P	1.658360	0.532553	-0.559318
P	-1.637000	0.336768	-0.477040
C	-0.721237	1.124268	-1.913292
C	0.679785	0.543124	-2.143977
H	-1.332855	1.046129	-2.824923
H	-0.650744	2.195192	-1.669120
H	0.624077	-0.504321	-2.482924
H	1.213627	1.117816	-2.917592
C	3.289068	-0.182782	-0.969355
C	3.569717	-0.819286	-2.189382
C	4.279227	-0.155524	0.032183
C	4.817304	-1.417083	-2.400625
H	2.827860	-0.852654	-2.989397
C	5.524839	-0.744159	-0.186744
H	4.078340	0.344143	0.984118
C	5.795028	-1.381018	-1.403797
H	5.025329	-1.907688	-3.354688
H	6.287269	-0.708474	0.595275
H	6.768899	-1.846270	-1.574191
C	1.964730	2.317633	-0.238687
C	3.113681	2.980904	-0.703967
C	0.990640	3.049859	0.465368
C	3.280289	4.347977	-0.466653
H	3.883937	2.432280	-1.250200
C	1.155879	4.418949	0.690114
H	0.089322	2.555957	0.833880
C	2.303745	5.069427	0.228131
H	4.178601	4.853101	-0.830203
H	0.386310	4.974198	1.231898
H	2.438731	6.138401	0.410327
C	-2.756062	-0.900846	-1.241950
C	-3.955454	-1.233851	-0.587493
C	-2.385836	-1.612272	-2.395747
C	-4.764777	-2.260537	-1.078474
H	-4.264281	-0.687563	0.306893
C	-3.199474	-2.638903	-2.883552
H	-1.461368	-1.377028	-2.927367
C	-4.387387	-2.968422	-2.224447
H	-5.695910	-2.507595	-0.562725
H	-2.902932	-3.182620	-3.783881
H	-5.021133	-3.772533	-2.605925
C	-2.763237	1.667284	0.087599
C	-3.651327	2.273131	-0.820250
C	-2.734487	2.103599	1.420454
C	-4.488197	3.306487	-0.397458
H	-3.696073	1.930086	-1.857097
C	-3.576174	3.139430	1.840719
H	-2.057561	1.633634	2.133010
C	-4.450651	3.741784	0.933198
H	-5.176129	3.772346	-1.107205

^{4}TS9-10A-19
Geometry with 77 atoms:
Total energy: -3045.568580240

Cr	-0.021609	-0.830814	1.256009
P	1.730032	0.273904	-0.431024
P	-1.562174	0.291921	-0.481850
C	-0.547575	0.826016	-1.970534
C	0.820998	0.139181	-2.052055
H	-1.127429	0.644170	-2.887454
H	-0.417111	1.914903	-1.882836
H	0.711582	-0.936606	-2.267071
H	1.421328	0.582254	-2.862162
C	3.335310	-0.563806	-0.696452
C	3.666796	-1.241500	-1.881195
C	4.242150	-0.585747	0.380782
C	4.880704	-1.930087	-1.982774
H	2.988481	-1.242048	-2.736336
C	5.455437	-1.265684	0.271720
H	4.002640	-0.060163	1.309387
C	5.775127	-1.944752	-0.909944
H	5.127763	-2.454234	-2.909307
H	6.153355	-1.269223	1.112536
H	6.722401	-2.482816	-0.993390
C	2.136933	2.067775	-0.345325
C	3.362838	2.573232	-0.813568
C	1.173278	2.966286	0.150078
C	3.614957	3.947254	-0.785195
H	4.125555	1.895590	-1.202547
C	1.426348	4.340437	0.167405
H	0.213066	2.603892	0.520791
C	2.649016	4.833336	-0.297370
H	4.572185	4.327097	-1.150887
H	0.664802	5.023998	0.550441
H	2.850516	5.907143	-0.278611
C	-2.834582	-0.829000	-1.178799
C	-4.151118	-0.803110	-0.690257
C	-2.467767	-1.808693	-2.118680
C	-5.082558	-1.745389	-1.134196
H	-4.453720	-0.049278	0.039654
C	-3.403496	-2.747244	-2.559784
H	-1.448169	-1.851594	-2.510372
C	-4.711484	-2.720516	-2.064856
H	-6.104614	-1.716200	-0.748877
H	-3.109092	-3.503359	-3.291583
H	-5.441702	-3.457520	-2.407352
C	-2.483654	1.798300	0.005943
C	-3.014279	2.666136	-0.966307
C	-2.675317	2.087964	1.365997
C	-3.707515	3.813661	-0.578199
H	-2.894788	2.448383	-2.030357
C	-3.375410	3.236424	1.750217
H	-2.280140	1.414924	2.126851
C	-3.886723	4.101971	0.780090
H	-4.114192	4.484159	-1.339216

H	-3.519086	3.453493	2.811432
H	-4.430341	5.001225	1.080134
C	1.414771	-2.212767	2.249781
C	1.416732	-3.025948	0.936868
C	0.074439	-3.299007	0.220450
C	-1.012278	-3.973577	1.086441
C	-2.130678	-3.012325	1.509772
C	-1.638320	-1.733836	2.198267
H	2.458627	-2.125207	2.570660
H	0.854229	-2.743840	3.028607
H	2.138945	-2.603310	0.224148
H	1.829790	-4.013475	1.216983
H	-0.346699	-2.383648	-0.259971
H	0.312030	-3.916953	-0.660026
H	-0.535107	-4.416120	1.978073
H	-1.454403	-4.816019	0.531184
H	-2.708278	-2.747122	0.610804
H	-2.839681	-3.554559	2.164116
H	-2.466271	-1.008839	2.293325
H	-1.287040	-1.947383	3.224497
C	0.191740	0.591629	2.783633
C	1.258194	-0.261535	3.151388
H	-0.708886	0.587931	3.403856
H	0.434290	1.542444	2.303220
H	2.274898	0.037964	2.883756
H	1.192929	-0.828368	4.082740

H	-4.125502	3.002178	2.694940
H	-4.782665	4.764731	1.055856
C	1.464442	-2.064453	2.219894
C	1.265020	-2.995298	0.980335
C	-0.118466	-3.211404	0.325694
C	-1.208286	-3.858175	1.186669
C	-1.559143	-3.055177	2.445874
C	-1.753241	-1.564879	2.148153
H	2.507610	-1.732193	2.193673
H	1.311012	-2.654610	3.128650
H	1.962058	-2.670696	0.193643
H	1.621599	-3.989570	1.303334
H	-0.530820	-2.280849	-0.132347
H	0.055188	-3.828769	-0.570699
H	-0.890916	-4.880387	1.456749
H	-2.110356	-3.965670	0.560179
H	-2.473957	-3.486845	2.894638
H	-0.774099	-3.194290	3.208126
H	-2.625006	-1.438370	1.483042
H	-1.973460	-1.007181	3.074332
C	0.253000	0.685220	2.687042
C	0.843869	-0.432890	3.348579
H	-0.738209	1.011127	3.014126
H	0.922164	1.491238	2.373112
H	1.889506	-0.364739	3.655839
H	0.223593	-0.991352	4.053685

H	-3.328043	4.287722	1.870638
H	-5.580471	4.274107	0.794985
C	-0.784221	-1.540201	2.821851
C	0.652426	-1.972510	3.040298
C	0.995181	-3.461193	2.931825
C	0.671445	-4.128938	1.590590
C	1.170524	-3.373566	0.348073
C	0.243253	-2.245930	-0.131942
H	-1.411033	-1.596082	3.714270
H	-1.317543	-2.085641	2.024538
H	1.353530	-1.432654	2.327860
H	0.996877	-1.579539	4.011011
H	2.075571	-3.566732	3.133695
H	0.476331	-3.994114	3.746848
H	-0.418313	-4.286204	1.498460
H	1.114933	-5.138055	1.611641
H	2.200099	-3.007815	0.519184
H	1.266539	-4.109679	-0.472176
H	0.506996	-1.993463	-1.170868
H	-0.781872	-2.650442	-0.185450
C	0.351790	1.178560	2.470322
C	-0.694798	0.505965	3.155728
H	0.114461	2.027294	1.828154
H	1.336414	1.244870	2.944894
H	-0.525913	0.238376	4.200986
H	-1.733096	0.790848	2.953248

^{4}TS9-10A-20
Geometry with 77 atoms:
Total energy: -3045.567450580

Cr	-0.058115	-0.746140	1.218748
P	1.741256	0.276743	-0.456966
P	-1.535197	0.335549	-0.576022
C	-0.498472	0.921383	-2.022216
C	0.869746	0.229815	-2.102550
H	-1.060250	0.778538	-2.957319
H	-0.359539	2.004754	-1.890378
H	0.766641	-0.832121	-2.377623
H	1.493244	0.712279	-2.871538
C	3.344285	-0.562866	-0.720716
C	3.685755	-1.221627	-1.913544
C	4.247601	-0.591944	0.359845
C	4.905536	-1.898852	-2.019626
H	3.012908	-1.212087	-2.773160
C	5.466426	-1.261545	0.246190
H	4.004173	-0.072073	1.290840
C	5.795823	-1.921587	-0.943335
H	5.161352	-2.406212	-2.953072
H	6.161930	-1.269410	1.088986
H	6.748448	-2.449390	-1.031214
C	2.158592	2.062875	-0.285747
C	3.407192	2.578685	-0.675447
C	1.177828	2.946992	0.202641
C	3.666256	3.948247	-0.573575
H	4.182900	1.913468	-1.060085
C	1.437828	4.316821	0.292135
H	0.203303	2.572641	0.520341
C	2.684535	4.819708	-0.091427
H	4.642149	4.336131	-0.876057
H	0.664020	4.988989	0.670823
H	2.892148	5.889670	-0.012867
C	-2.713656	-0.867839	-1.314135
C	-4.041922	-0.942067	-0.862487
C	-2.261172	-1.800140	-2.264810
C	-4.899371	-1.928914	-1.356922
H	-4.416309	-0.225062	-0.129028
C	-3.122473	-2.784026	-2.756764
H	-1.233826	-1.768916	-2.633023
C	-4.443062	-2.852538	-2.301859
H	-5.931822	-1.972226	-1.001922
H	-2.759338	-3.498459	-3.499598
H	-5.116280	-3.622281	-2.686618
C	-2.560742	1.769645	-0.083778
C	-2.947239	2.757665	-1.006846
C	-2.992274	1.866223	1.250473
C	-3.739171	3.831298	-0.593692
H	-2.637865	2.695909	-2.052483
C	-3.792849	2.937885	1.656183
H	-2.711022	1.097979	1.972069
C	-4.161976	3.923798	0.736953
H	-4.032131	4.596872	-1.316162

^{4}TS9-10A-21
Geometry with 77 atoms:
Total energy: -3045.561601230

Cr	0.066239	-0.500435	1.110173
P	1.567128	0.566463	-0.552374
P	-1.717119	0.236344	-0.501840
C	-0.836316	1.048174	-1.937085
C	0.604452	0.565597	-2.150272
H	-1.440406	0.924146	-2.848976
H	-0.853616	2.123989	-1.710450
H	0.617761	-0.466082	-2.529314
H	1.115331	1.202726	-2.888227
C	3.081381	-0.413202	-0.843537
C	3.495705	-0.840408	-2.114162
C	3.847609	-0.761591	0.284139
C	4.654899	-1.611222	-2.250408
H	2.925831	-0.577202	-3.007470
C	5.010031	-1.520933	0.142688
H	3.535173	-0.433661	1.280023
C	5.412528	-1.951387	-1.126398
H	4.968307	-1.943725	-3.243002
H	5.598831	-1.783533	1.024904
H	6.318014	-2.552509	-1.238588
C	2.145620	2.309412	-0.395623
C	3.505302	2.653247	-0.484414
C	1.201261	3.331177	-0.176550
C	3.906924	3.986953	-0.359783
H	4.259251	1.882554	-0.653500
C	1.605483	4.662715	-0.063130
H	0.138499	3.098651	-0.090540
C	2.961265	4.994121	-0.151548
H	4.968274	4.237641	-0.430112
H	0.857836	5.442516	0.101351
H	3.279173	6.035144	-0.056005
C	-2.652973	-1.184837	-1.169641
C	-3.538620	-1.847445	-0.298973
C	-2.437729	-1.702978	-2.454957
C	-4.209899	-2.996519	-0.717463
H	-3.707222	-1.462480	0.710945
C	-3.109429	-2.858493	-2.868353
H	-1.741517	-1.222783	-3.144834
C	-3.995462	-3.505373	-2.004055
H	-4.901116	-3.499085	-0.036641
H	-2.935429	-3.253685	-3.872052
H	-4.518049	-4.407898	-2.329862
C	-2.991677	1.479948	-0.053578
C	-4.262201	1.478353	-0.656227
C	-2.666235	2.499832	0.859018
C	-5.185996	2.480485	-0.348747
H	-4.536145	0.694826	-1.365459
C	-3.592648	3.502022	1.159020
H	-1.690370	2.519070	1.345338
C	-4.854377	3.493088	0.556931
H	-6.170761	2.469379	-0.822206

^{4}TS9-10B-01
Geometry with 85 atoms:
Total energy: -3274.483068060

Cr	-0.534934	-0.689184	1.055591
P	1.576358	-0.304888	-0.351180
P	-1.489834	0.393053	-0.987335
C	-0.346474	0.048023	-2.405225
C	1.093030	0.406809	-2.018623
H	-0.436761	-1.026977	-2.630832
H	-0.663269	0.605755	-3.300805
H	1.806244	0.046312	-2.771213
H	1.209063	1.498377	-1.974899
C	2.707010	-1.689670	-0.749791
C	2.431105	-2.997340	-0.327015
C	3.900776	-1.441314	-1.478027
C	3.311358	-4.047501	-0.603532
H	1.512983	-3.201129	0.221712
C	4.788477	-2.493094	-1.745612
C	4.487404	-3.786641	-1.308003
H	3.078345	-5.059476	-0.266407
H	5.710292	-2.311935	-2.298419
H	5.186712	-4.597610	-1.526676
C	2.669485	0.941367	0.451231
C	2.571821	2.318024	0.198707
C	3.577017	0.493445	1.427700
C	3.370294	3.226588	0.900716
H	1.870493	2.705855	-0.540670
C	4.371750	1.403018	2.129088
H	3.674653	-0.574705	1.635597
C	4.271965	2.773977	1.868153
H	3.284020	4.294893	0.686101
H	5.076677	1.037002	2.879744
H	4.897369	3.484917	2.413567
C	-1.313371	2.190795	-0.689880
C	-1.725052	3.134999	-1.644060
C	-0.740342	2.640425	0.519152
C	-1.570314	4.502205	-1.418234
H	-2.183928	2.784777	-2.572513
C	-0.585484	4.014993	0.750926
H	-0.999253	4.932744	-0.217467
C	-1.896220	5.225193	-2.168669
H	-0.137382	4.381744	1.672470
H	-0.871811	6.000473	-0.023106
C	-3.193578	0.167867	-1.595375
C	-4.249627	0.727405	-0.851760
C	-3.486437	-0.646754	-2.702028
C	-5.574436	0.476010	-1.212412
H	-4.036664	1.368032	0.007913
C	-4.815617	-0.894662	-3.057565
H	-2.686683	-1.099468	-3.291342
C	-5.860124	-0.338015	-2.314304
H	-6.387286	0.917519	-0.630781
H	-5.034135	-1.527540	-3.921114
H	-6.897601	-0.535823	-2.594239

O	4.099910	-0.166601	-1.878912
O	-0.337506	1.689048	1.433078
C	5.334069	0.216784	-2.463825
H	5.272884	1.301547	-2.623507
H	6.182254	-0.000710	-1.792442
H	5.498189	-0.281397	-3.434995
C	0.155207	2.137049	2.703754
H	1.093537	2.697005	2.581581
H	-0.598833	2.754618	3.215501
H	0.351977	1.242583	3.301299
C	-2.237310	-0.504163	2.464875
C	-3.319449	-1.358546	3.110101
C	-4.058539	-2.320990	2.173967
C	-3.243822	-3.418791	1.469104
C	-2.492800	-3.028569	0.179197
C	-1.043288	-2.550251	0.315669
H	-2.069852	0.430719	3.016593
H	-2.598710	-0.222508	1.456022
H	-2.920888	-1.919506	3.975139
H	-4.072589	-0.675105	3.543962
H	-4.845101	-2.810526	2.773417
H	-4.594498	-1.734745	1.404717
H	-3.958385	-4.213765	1.198245
H	-2.544178	-3.890370	2.183948
H	-2.479498	-3.925239	-0.470083
H	-3.098591	-2.291675	-0.376420
H	-0.483260	-3.269022	0.942821
H	-0.562968	-2.573128	-0.680413
C	0.763634	-1.350491	2.631441
C	-0.487794	-1.515179	3.259518
H	1.433558	-0.552153	2.966363
H	1.267762	-2.229358	2.222392
H	-0.948231	-2.504728	3.243944
H	-0.726127	-0.933687	4.153338

^{4}TS9-10B-02
Geometry with 85 atoms:
Total energy: -3274.481313740

Cr	-0.305063	-0.556061	1.016659
P	1.584067	0.063015	-0.660966
P	-1.621802	0.450147	-0.863518
C	-0.652638	0.270440	-2.430314
C	0.776476	0.771536	-2.197400
H	-0.670907	-0.798877	-2.692431
H	-1.136285	0.826296	-3.249060
H	1.411731	0.590960	-3.077136
H	0.766703	1.860474	-2.034457
C	2.533542	-1.382673	-1.277110
C	2.255461	-2.018476	-2.494647
C	3.545694	-1.920632	-0.445049
C	2.962605	-3.156758	-2.894428
H	1.477307	-1.629933	-3.153765
C	4.262995	-3.055102	-0.847838
C	3.964011	-3.668153	-2.068430
H	2.730526	-3.637189	-3.847104
H	5.048834	-3.466910	-0.214806
H	4.524900	-4.555923	-2.370813
C	2.858787	1.336248	-0.304229
C	2.869134	1.989190	0.935231
C	3.819375	1.675573	-1.270931
C	3.819995	2.977484	1.205458
H	2.138692	1.711606	1.693118
C	4.768812	2.663609	-0.999770
H	3.835653	1.159639	-2.234589
C	4.769720	3.317436	0.237721
H	3.823183	3.479748	2.176351
H	5.514183	2.921668	-1.756150
H	5.514716	4.088810	0.448065
C	-1.576728	2.248672	-0.521848
C	-2.106534	3.176315	-1.432983
C	-0.978640	2.719558	0.665863
C	-2.039121	4.547017	-1.187436
H	-2.588984	2.810267	-2.343301
C	-0.910309	4.096886	0.917302
C	-1.435691	4.998739	-0.010813
H	-2.455677	5.256842	-1.904946
H	-0.447249	4.479449	1.825329
H	-1.372429	6.069560	0.196964
C	-3.361062	0.074811	-1.261067
C	-4.364522	0.530165	-0.385575
C	-3.713984	-0.748201	-2.344305
C	-5.696996	0.169765	-0.594452
H	-4.106184	1.176390	0.457200
C	-5.050296	-1.104172	-2.548282
H	-2.954988	-1.122013	-3.034595
C	-6.042363	-0.649368	-1.674929
H	-6.469283	0.531932	0.088492
H	-5.315736	-1.740887	-3.395710
H	-7.085554	-0.930933	-1.837061
O	3.752354	-1.266497	0.720860
O	-0.474478	1.786640	1.554941
C	4.783719	-1.672245	1.603423
H	4.765814	-0.962944	2.441585
H	4.611431	-2.691840	1.989887
H	5.772698	-1.626671	1.115943
C	-0.199430	2.224933	2.892121
H	0.065648	1.334976	3.471362
H	0.644053	2.931293	2.915252
H	-1.090939	2.695411	3.335123
C	-1.946785	-0.786729	2.509261
C	-2.819129	-1.881627	3.109865
C	-3.395193	-2.902672	2.122547
C	-2.415078	-3.782884	1.327845
C	-1.806085	-3.182542	0.044912
C	-0.477406	-2.428620	0.155944
H	-1.935780	0.110504	3.142363
H	-2.409828	-0.489866	1.549146
H	-2.288223	-2.414126	3.920393
H	-3.673783	-1.390466	3.610922
H	-4.057872	-3.567765	2.702447
H	-4.055772	-2.378678	1.406972
H	-2.976930	-4.682775	1.026748
H	-1.610768	-4.153957	1.990191
H	-1.640261	-4.023589	-0.656120
H	-2.572356	-2.556612	-0.446697
H	0.265501	-3.054364	0.685241
H	-0.069947	-2.291979	-0.861651
C	1.152339	-1.069989	2.497715
C	-0.010087	-1.507826	3.160241
H	1.689607	-0.190826	2.866900
H	1.770645	-1.795897	1.968134
H	-0.286378	-2.560210	3.076309
H	-0.302697	-1.051945	4.109315

^{4}TS9-10B-03
Geometry with 85 atoms:
Total energy: -3274.483582580

Cr	-0.076255	0.084696	1.313708
P	1.642171	0.494402	-0.672613
P	-1.591171	-0.011964	-0.697089
C	-0.741303	0.752200	-2.163627
C	0.719322	0.305310	-2.277787
H	-1.307587	0.527648	-3.080619
H	-0.819175	1.835626	-1.998022
H	0.784460	-0.766867	-2.509403
H	1.246199	0.840797	-3.082585
C	3.105841	-0.590153	-0.896490
C	4.421895	-0.128589	-1.034678
C	2.869104	-1.987433	-0.895110
C	5.489263	-1.024922	-1.148226
H	4.620821	0.944059	-1.057069
C	3.936751	-2.886970	-1.007764
C	5.241925	-2.398178	-1.128995
H	6.508351	-0.647192	-1.254261
H	3.761347	-3.962455	-1.007670
H	6.069732	-3.106354	-1.215296
C	2.288108	2.211788	-0.655354
C	3.131587	2.599602	0.404249
C	1.875058	3.186187	-1.579009
C	3.561061	3.921837	0.526811
H	3.466332	1.859646	1.134846
C	2.298128	4.513554	-1.447477
H	1.216413	2.926930	-2.409233
C	3.140502	4.885204	-0.396886
H	4.223419	4.202455	1.349390
H	1.968145	5.258385	-2.175897
H	3.471295	5.921839	-0.298124
C	-3.250984	0.771797	-0.663708
C	-4.436091	0.040867	-0.828627
C	-3.336590	2.163935	-0.413004
C	-5.684979	0.662047	-0.738031
H	-4.388509	-1.029902	-1.032173
C	-4.588535	2.786215	-0.318548
C	-5.754440	2.031006	-0.478726
H	-6.596134	0.075085	-0.870503
H	-4.663512	3.855579	-0.123018
H	-6.725021	2.527236	-0.402000
C	-1.912163	-1.760256	-1.178693
C	-1.688234	-2.260206	-2.472052
C	-2.397104	-2.635804	-0.189118
C	-1.936426	-3.605345	-2.764311
H	-1.321486	-1.611963	-3.269364
C	-2.657673	-3.975574	-0.486745
H	-2.586185	-2.265157	0.818240
C	-2.422624	-4.465627	-1.775844
H	-1.754165	-3.979244	-3.774846
H	-3.043555	-4.637405	0.292548
H	-2.620099	-5.514637	-2.009600
O	1.565978	-2.361018	-0.792659
O	-2.155268	2.821110	-0.294006
C	1.222030	-3.736090	-0.710452
H	0.134858	-3.775379	-0.578880
H	1.490955	-4.273614	-1.635278
H	1.712311	-4.223989	0.149596
C	-2.137192	4.212958	-0.020702
H	-1.080373	4.504766	0.031453
H	-2.628971	4.787866	-0.824362
H	-2.622134	4.443330	0.943198
C	1.641769	-0.211715	2.686510
C	1.260987	-1.642344	2.277037
C	0.803109	-2.550653	3.422672
C	-0.405954	-2.053587	4.221753
C	-1.647477	-1.761507	3.367545
C	-1.628872	-0.409181	2.642599
H	2.571900	0.093225	2.195434
H	1.784224	-0.175946	3.770746
H	0.489915	-1.743259	1.448690
H	2.132115	-2.083270	1.768819
H	0.570676	-3.544618	3.001524
H	1.660668	-2.696631	4.101551
H	-0.137003	-1.146977	4.793754
H	-0.645560	-2.820873	4.976487
H	-1.781751	-2.596512	2.654499
H	-2.536205	-1.802144	4.025850
H	-2.576621	-0.267088	2.092061
H	-1.618557	0.389177	3.406681
C	-0.126197	2.088714	1.839968
C	0.766127	1.647955	2.862165
H	-1.169756	2.280334	2.100736
H	0.275033	2.713638	1.038197
H	1.776262	2.064352	2.876811
H	0.347984	1.487225	3.858893

^{4}TS9-10B-04
Geometry with 85 atoms:
Total energy: -3274.479727900

Cr	-0.259578	-0.405818	1.085419
P	1.604362	0.144837	-0.661582
P	-1.636240	0.379962	-0.872636
C	-0.629553	0.251337	-2.425661
C	0.761351	0.844747	-2.177565
H	-0.569268	-0.815404	-2.689994
H	-1.144126	0.771423	-3.249092
H	1.412681	0.731469	-3.057651
H	0.683116	1.926406	-1.984019
C	2.514419	-1.321656	-1.284861
C	2.259539	-1.920667	-2.525611
C	3.476633	-1.912608	-0.428889
C	2.938223	-3.077271	-2.922821
H	1.524453	-1.488644	-3.206168
C	4.165895	-3.064968	-0.828863
C	3.888277	-3.642573	-2.071776
H	2.725131	-3.528976	-3.893807
H	4.913920	-3.517450	-0.178111
H	4.426714	-4.544764	-2.372325
C	2.909302	1.400134	-0.355696
C	2.770315	2.291375	0.717352
C	4.027729	1.504790	-1.198632
C	3.730825	3.281720	0.943438
H	1.909723	2.204769	1.378823
C	4.987240	2.493669	-0.969952
H	4.156962	0.805932	-2.028952
C	4.840333	3.384353	0.099649

H 3.615512 3.970793 1.784122
H 5.855904 2.568010 -1.629008
H 5.594086 4.155641 0.276433
C -1.841854 2.186544 -0.665526
C -2.515932 2.956848 -1.627284
C -1.282540 2.829620 0.458794
C -2.642835 4.337970 -1.485917
H -2.958311 2.457362 -2.493013
C -1.411880 4.218183 0.606178
C -2.086846 4.960550 -0.365562
H -3.171892 4.922918 -2.240943
H -0.988117 4.734965 1.465437
H -2.176729 6.041951 -0.237770
C -3.289699 -0.281385 -1.262712
C -4.434366 0.278675 -0.667515
C -3.416601 -1.456659 -2.025282
C -5.682381 -0.325007 -0.837455
H -4.354892 1.191027 -0.072104
C -4.668320 -2.054042 -2.192510
H -2.542831 -1.919896 -2.488747
C -5.802371 -1.492447 -1.597608
H -6.565341 0.120114 -0.372435
H -4.755933 -2.965214 -2.789139
H -6.779312 -1.964154 -1.727548
O 3.664988 -1.286684 0.755151
O -0.614040 2.051591 1.384309
C 4.654085 -1.744381 1.661448
H 4.631114 -1.054969 2.515518
H 4.438294 -2.766716 2.017536
H 5.659009 -1.718886 1.206197
C -0.332575 2.638438 2.660421
H 0.122851 1.858440 3.276914
H 0.379400 3.473137 2.570124
H -1.259981 2.990293 3.139188
C -1.893533 -0.466884 2.656334
C -2.783086 -1.668910 2.959638
C -3.170713 -2.535708 1.748072
C -2.273954 -3.745237 1.460511
C -0.764555 -3.489063 1.376493
C -0.324604 -2.378658 0.420135
H -1.958821 0.280551 3.455510
H -2.292266 0.052045 1.763706
H -2.336764 -2.298468 3.751803
H -3.710604 -1.269756 3.409571
H -4.196779 -2.912256 1.894564
H -3.227425 -1.893927 0.855055
H -2.609939 -4.194125 0.508165
H -2.450689 -4.514447 2.233954
H -0.362119 -3.312177 2.388624
H -0.290545 -4.438634 1.061140
H 0.724648 -2.543103 0.128627
H -0.921129 -2.426357 -0.510022
C 1.217108 -0.731613 2.589405
C 0.091016 -0.874787 3.423698
H 1.852215 0.155464 2.685731
H 1.724603 -1.622043 2.212978
H -0.244447 -1.873638 3.706201
H -0.086194 -0.126874 4.199272

^{4}TS9-10B-05
Geometry with 85 atoms:
Total energy: -3274.480729800
Cr -0.542743 -0.735536 1.023035
P 1.553500 -0.249876 -0.388132
P -1.518873 0.480213 -0.950470
C -0.394596 0.215305 -2.399408
C 1.054487 0.537141 -2.016713
H -0.499099 -0.843382 -2.687864
H -0.718420 0.827129 -3.256189
H 1.751901 0.198916 -2.793884
H 1.191423 1.623733 -1.926163
C 2.669027 -1.626391 -0.846903
C 2.401565 -2.939184 -0.434905
C 3.845586 -1.368624 -1.599285
C 3.269547 -3.987777 -0.752450
H 1.500765 -3.145501 0.141137
C 4.720364 -2.419489 -1.909976
C 4.425425 -3.719315 -1.486959
H 3.043254 -5.004131 -0.424126
H 5.627832 -2.232665 -2.484257
H 5.114539 -4.529124 -1.739616
C 2.660656 0.960589 0.447460
C 3.659301 0.478560 1.312582
C 2.474479 2.347025 0.334939
C 4.455688 1.365223 2.041094
H 3.827436 -0.596457 1.411043
C 3.273759 3.232370 1.064884
H 1.705170 2.759170 -0.318460
C 4.265914 2.745993 1.920786
H 5.232183 0.973676 2.703009
H 3.117196 4.308951 0.958684
H 4.892102 3.438815 2.488169
C -1.346866 2.259907 -0.558834
C -1.715763 3.247528 -1.486396
C -0.829942 2.651751 0.693936
C -1.572254 4.602797 -1.193054
H -2.130739 2.941695 -2.450435
C -0.688544 4.015168 0.994061
C -1.057811 4.977102 0.051111
H -1.863310 5.359368 -1.924407
H -0.283518 4.340594 1.950119
H -0.939987 6.034526 0.300074
C -3.228190 0.296890 -1.559718
C -4.274650 0.766398 -0.743861
C -3.534440 -0.401211 -2.739185
C -5.603647 0.544387 -1.106773
H -4.049996 1.312335 0.176377
C -4.868223 -0.620174 -3.097268
H -2.742266 -0.787579 -3.383362
C -5.903205 -0.151402 -2.283534
H -6.409222 0.915691 -0.468612
H -5.097681 -1.162469 -4.017816
H -6.944074 -0.326942 -2.565787
O 4.044317 -0.086180 -1.975191
O -0.464092 1.659553 1.580188
C 5.270653 0.303601 -2.572675
H 5.214028 1.392255 -2.704924
H 6.128544 0.064085 -1.921422
H 5.414328 -0.171391 -3.558537
C 0.002895 2.066702 2.873223
H 0.936462 2.641907 2.786900
H -0.766078 2.657097 3.395231
H 0.201376 1.157382 3.444580
C -2.274929 -0.833735 2.406249
C -3.140686 -1.937693 3.011911
C -2.928396 -3.371708 2.503475
C -3.267587 -3.681562 1.040301
C -2.571552 -2.843331 -0.047949
C -1.074229 -2.550093 0.159500
H -2.356527 0.099880 2.981636
H -2.646416 -0.599558 1.391406
H -2.993568 -1.940711 4.106419
H -4.202483 -1.661677 2.864299
H -1.885699 -3.676427 2.690272
H -3.536682 -4.041089 3.135750
H -4.359389 -3.599748 0.892846
H -3.023261 -4.746398 0.876470
H -2.712771 -3.375341 -1.006889
H -3.136587 -1.907784 -0.182043
H -0.595510 -3.341988 0.764206
H -0.551266 -2.543409 -0.813039
C 0.837340 -1.297643 2.568808
C -0.359971 -1.432944 3.296003
H 1.490602 -0.439135 2.753213
H 1.346166 -2.200599 2.219826
H -0.731638 -2.437603 3.489478
H -0.601730 -0.718240 4.086047

^{4}TS9-10B-06
Geometry with 85 atoms:
Total energy: -3274.479601830
Cr -0.108302 -0.006635 1.098637
P 1.662787 0.288121 -0.755535
P -1.597609 0.217719 -0.950319
C -0.557546 0.228785 -2.489101
C 0.747759 0.988306 -2.222869
H -0.353104 -0.818369 -2.758426
H -1.124166 0.683207 -3.316680
H 1.395247 1.009293 -3.112554
H 0.533087 2.039976 -1.973978
C 2.436426 -1.250512 -1.394445
C 2.377796 -1.632167 -2.743420
C 3.064652 -2.124872 -0.473026
C 2.898632 -2.854254 -3.177042
H 1.922532 -0.972067 -3.482368
C 3.580385 -3.355631 -0.904153
C 3.489999 -3.714573 -2.251375
H 2.840838 -3.128009 -4.232481
H 4.054883 -4.035746 -0.197517
H 3.895119 -4.676297 -2.575547
C 3.029151 1.486075 -0.500918
C 4.378355 1.100558 -0.501639
C 2.701052 2.829034 -0.239050
C 5.379001 2.043922 -0.248467
H 4.655808 0.065696 -0.706742
C 3.703606 3.769416 0.005243
H 1.656588 3.147440 -0.233724
C 5.046710 3.377408 0.005039
H 6.426410 1.732305 -0.254957
H 3.435925 4.811672 0.196836
H 5.832450 4.111431 0.199182
C -2.308798 1.904587 -0.897852
C -3.362911 2.278240 -1.746972
C -1.798586 2.849090 0.017841
C -3.919115 3.555899 -1.689366
H -3.762883 1.545435 -2.452012
C -2.365428 4.130157 0.087905
C -3.418298 4.473749 -0.764288
H -4.740677 3.828864 -2.354645
H -2.000964 4.869692 0.798113
H -3.848329 5.475869 -0.696062
C -3.012875 -0.888750 -1.265063
C -4.178080 -0.731021 -0.490574
C -2.913012 -1.985928 -2.136617
C -5.223395 -1.649988 -0.594722
H -4.272755 0.113895 0.195962
C -3.963444 -2.902951 -2.236181
H -2.015946 -2.143596 -2.738275
C -5.118242 -2.739274 -1.466314
H -6.124124 -1.515122 0.008999
H -3.875841 -3.750753 -2.919897
H -5.936111 -3.459553 -1.544634
O 3.147349 -1.681532 0.801973
O -0.737763 2.463450 0.814106
C 3.730360 -2.503872 1.800832
H 4.790862 -2.715558 1.581087
H 3.671720 -1.941006 2.741753
H 3.180782 -3.453753 1.914905
C -0.224778 3.431345 1.735877
H 0.075390 4.353003 1.214253
H -0.969669 3.670219 2.511473
H 0.663055 2.995302 2.199536
C -1.698511 -0.002461 2.672084
C -2.090457 -0.996167 3.766558
C -1.346929 -2.340486 3.790863
C -1.636357 -3.332917 2.659356
C -1.400396 -2.846932 1.219960
C -0.095747 -2.078424 0.969384
H -2.105587 0.999223 2.871675
H -2.148826 -0.327492 1.716492
H -1.952347 -0.509134 4.747940
H -3.177774 -1.190867 3.692976
H -0.260068 -2.155058 3.824266
H -1.585450 -2.841012 4.745067
H -2.679968 -3.685990 2.742320
H -1.004205 -4.221152 2.839515
H -1.431038 -3.737706 0.564916
H -2.269514 -2.253492 0.894079
H 0.716431 -2.412829 1.638148
H 0.254354 -2.260174 -0.060364
C 1.407162 0.469174 2.531726
C 0.314249 0.500706 3.412956
H 1.878078 1.395927 2.189035
H 2.060180 -0.403727 2.523088
H 0.208103 -0.297252 4.145344
H -0.077952 1.461956 3.752763

^{4}TS9-10B-07
Geometry with 85 atoms:
Total energy: -3274.479495860
Cr 0.221453 -0.778092 1.008968
P -1.713434 0.498372 -0.496948
P 1.561146 0.578544 -0.658112

C	0.532937	1.479336	-1.925989
C	-0.830942	0.806889	-2.114870
H	0.414392	2.510063	-1.568865
H	1.076933	1.506368	-2.882445
H	-1.470894	1.409126	-2.777810
H	-0.697924	-0.180228	-2.582814
C	-2.526392	2.120874	-0.121116
C	-3.900624	2.320868	-0.330236
C	-1.763842	3.201357	0.389286
C	-4.515756	3.539753	-0.032853
H	-4.508398	1.510037	-0.733713
C	-2.379460	4.424630	0.688609
C	-3.751698	4.587333	0.479852
H	-5.586694	3.665051	-0.205859
H	-1.795388	5.256681	1.080460
H	-4.218660	5.546122	0.718112
C	-3.131628	-0.576047	-0.961352
C	-3.975118	-1.023039	0.074326
C	-3.388884	-1.008553	-2.273198
C	-5.041192	-1.883654	-0.192425
H	-3.810776	-0.677303	1.097957
C	-4.452482	-1.878562	-2.537307
H	-2.769471	-0.674187	-3.106445
C	-5.278277	-2.320266	-1.500541
H	-5.687553	-2.215394	0.623776
H	-4.638439	-2.205944	-3.563266
H	-6.108703	-2.998489	-1.711002
C	2.323681	-0.770243	-1.645749
C	3.581289	-0.682290	-2.254252
C	1.597491	-1.974024	-1.748469
C	4.105597	-1.764180	-2.968000
H	4.158544	0.240775	-2.162433
C	2.112231	-3.058702	-2.462122
C	3.368049	-2.944290	-3.070132
H	5.087869	-1.683985	-3.438278
H	1.559953	-3.994319	-2.541227
H	3.769930	-3.796970	-3.622505
C	2.915608	1.718733	-0.219650
C	3.565727	1.534643	1.013823
C	3.301220	2.786049	-1.049527
C	4.586379	2.403163	1.407863
H	3.270497	0.712805	1.668957
C	4.318905	3.655742	-0.647539
H	2.811727	2.948978	-2.011773
C	4.961724	3.466499	0.580028
H	5.086074	2.251852	2.367707
H	4.611222	4.484265	-1.297362
H	5.756155	4.148835	0.892019
O	-0.428700	2.986325	0.550162
O	0.374477	-2.013277	-1.096841
C	0.400015	4.010832	1.086099
H	0.059482	4.321232	2.088188
H	1.406910	3.583326	1.165044
H	0.432018	4.889222	0.419501
C	-0.547662	-3.051389	-1.457345
H	-0.192554	-4.035965	-1.116671
H	-1.497897	-2.819355	-0.964921
H	-0.699346	-3.064720	-2.547404
C	-1.115109	-2.180162	2.003406
C	-0.981066	-3.146438	3.177997
C	0.417103	-3.340463	3.779320
C	1.475315	-4.019580	2.901294
C	1.825422	-3.341230	1.562789
C	1.944704	-1.808217	1.609706
H	-2.170192	-1.964096	1.797834
H	-0.714826	-2.666243	1.091946
H	-1.662060	-2.815992	3.981827
H	-1.373647	-4.132297	2.860203
H	0.805327	-2.364545	4.115704
H	0.307238	-3.941717	4.698058
H	1.170190	-5.063052	2.703765
H	2.397759	-4.087072	3.505013
H	2.776776	-3.779200	1.209196
H	1.093915	-3.650035	0.795345
H	2.247030	-1.466615	2.614659
H	2.744011	-1.483385	0.923887
C	0.219778	0.632565	2.619373
C	-0.771073	-0.223503	3.105539
H	-0.065556	1.547685	2.101259
H	1.215354	0.610268	3.069861
H	-0.576228	-0.843176	3.979513
H	-1.822688	0.031050	2.949279

^{4}TS9-10B-08
Geometry with 85 atoms:
Total energy: -3274.481570770

Cr	-0.246384	-0.436287	1.110187
P	1.617272	0.101462	-0.661239
P	-1.628891	0.315888	-0.853509
C	-0.640714	0.147695	-2.411743
C	0.755731	0.743308	-2.193912
H	-0.592297	-0.926462	-2.649326
H	-1.157566	0.651266	-3.243995
H	1.398616	0.597988	-3.075248
H	0.680518	1.831269	-2.039799
C	2.549024	-1.366643	-1.251023
C	2.289434	-1.998098	-2.475342
C	3.531386	-1.924682	-0.396094
C	2.978259	-3.154552	-2.854407
H	1.543544	-1.590403	-3.158842
C	4.232360	-3.075915	-0.778792
C	3.946675	-3.687407	-2.003206
H	2.759357	-3.630863	-3.812224
H	4.995506	-3.501770	-0.127551
H	4.493545	-4.589122	-2.289556
C	2.890025	1.397592	-0.389104
C	4.122940	1.390581	-1.060655
C	2.593770	2.446585	0.493680
C	5.041625	2.421361	-0.848291
H	4.370835	0.576195	-1.745567
C	3.511947	3.479881	0.700192
H	1.640051	2.448512	1.019869
C	4.738900	3.467418	0.030661
H	6.000187	2.407937	-1.373127
H	3.270684	4.293520	1.389026
H	5.461005	4.271271	0.193913
C	-1.764659	2.133718	-0.644405
C	-2.369263	2.929361	-1.630950
C	-1.242665	2.754232	0.508284
C	-2.451382	4.314077	-1.491589
H	-2.790489	2.448003	-2.517506
C	-1.324532	4.146277	0.654519
C	-1.924442	4.914949	-0.345703
H	-2.925196	4.918662	-2.267538
H	-0.923697	4.644439	1.535643
H	-1.979518	5.998773	-0.219263
C	-3.329604	-0.227199	-1.232796
C	-3.609976	-1.135741	-2.266664
C	-4.371774	0.199130	-0.388268
C	-4.912314	-1.610144	-2.449562
H	-2.819877	-1.486020	-2.933376
C	-5.669764	-0.277962	-0.576229
H	-4.169984	0.910834	0.416584
C	-5.942224	-1.186092	-1.605298
H	-5.120909	-2.315438	-3.257640
H	-6.472344	0.060605	0.083469
H	-6.958203	-1.561072	-1.750001
O	3.733729	-1.267102	0.768825
O	-0.654092	1.947588	1.466320
C	4.769200	-1.666228	1.651794
H	4.754743	-0.950445	2.484303
H	4.598617	-2.682458	2.047176
H	5.755242	-1.625001	1.158181
C	-0.408544	2.522008	2.757543
H	-0.060729	1.714605	3.407045
H	0.372514	3.296708	2.709353
H	-1.333899	2.950460	3.171995
C	-1.863838	-0.661278	2.615891
C	-2.563479	-1.834137	3.288888
C	-2.479377	-3.184690	2.556039
C	-2.788215	-3.102831	1.046206
C	-1.558345	-3.170059	0.118069
C	-0.286995	-2.426008	0.538978
H	-2.023384	0.271215	3.174713
H	-2.337201	-0.509546	1.627720
H	-2.205779	-1.953034	4.327221
H	-3.633162	-1.562838	3.382579
H	-1.483949	-3.635106	2.708404
H	-3.185918	-3.872014	3.048786
H	-3.358851	-2.181582	0.840595
H	-3.467185	-3.922179	0.759716
H	-1.287784	-4.237898	-0.005334
H	-1.871167	-2.840442	-0.887922
H	0.171262	-2.921660	1.412914
H	0.454504	-2.520618	-0.271080
C	1.275518	-0.594215	2.625307
C	0.175577	-0.981225	3.403592
H	1.737922	0.388997	2.767731
H	1.928428	-1.356055	2.198412
H	-0.011908	-2.045808	3.550903
H	-0.167262	-0.355063	4.230566

^{4}TS9-10B-09
Geometry with 85 atoms:
Total energy: -3274.479925890

Cr	-0.280974	-0.680774	1.214168
P	1.316257	0.520348	-0.641155
P	-1.810030	-0.160480	-0.629145
C	-0.900949	-0.303100	-2.238746
C	0.328875	0.611587	-2.239619
H	-0.601295	-1.356050	-2.335225
H	-1.570971	-0.059544	-3.078383
H	0.983636	0.376202	-3.089070
H	0.003267	1.656312	-2.342892
C	2.941081	-0.236583	-1.065642
C	4.138103	0.305352	-0.573610
C	2.994833	-1.453436	-1.786384
C	5.362404	-0.336142	-0.780501
H	4.117423	1.244149	-0.016959
C	4.221525	-2.097711	-1.995566
C	5.398208	-1.537415	-1.488967
H	6.281344	0.105516	-0.389471
H	4.267880	-3.032782	-2.553529
H	6.348695	-2.049649	-1.657281
C	1.761164	2.278124	-0.311784
C	1.955616	3.207309	-1.349342
C	1.934331	2.703458	1.015369
C	2.285602	4.533608	-1.061575
H	1.859508	2.901731	-2.393439
C	2.273923	4.028743	1.302894
H	1.812135	1.996536	1.836661
C	2.440588	4.949383	0.264877
H	2.428619	5.244683	-1.878908
H	2.409443	4.341122	2.341518
H	2.699753	5.987388	0.487425
C	-2.202209	1.620631	-0.506690
C	-2.900715	2.286284	-1.526526
C	-1.740528	2.357457	0.604354
C	-3.136362	3.658684	-1.460411
H	-3.269816	1.712325	-2.380441
C	-1.973817	3.738704	0.672780
C	-2.664587	4.377985	-0.358565
H	-3.682348	4.163448	-2.260001
H	-1.612114	4.326526	1.514616
H	-2.834904	5.455375	-0.294108
C	-3.396283	-1.029263	-0.856596
C	-3.470139	-2.190282	-1.646163
C	-4.535112	-0.602687	-0.150231
C	-4.667631	-2.906343	-1.731444
H	-2.597563	-2.542438	-2.199967
C	-5.728325	-1.322173	-0.240543
H	-4.493557	0.300509	0.463500
C	-5.797117	-2.475336	-1.029730
H	-4.716636	-3.804898	-2.351381
H	-6.609702	-0.979317	0.306993
H	-6.732140	-3.036438	-1.099039
O	1.808198	-1.930206	-2.246090
O	-1.062896	1.675382	1.591987
C	1.750987	-3.197905	-2.879701
H	2.122726	-3.999375	-2.218777
H	0.692273	-3.385493	-3.103943
H	2.322343	-3.205073	-3.823652
C	-0.929909	2.312358	2.866669
H	-0.509239	1.570877	3.553437
H	-0.248137	3.174394	2.813880
H	-1.913775	2.634754	3.242914
C	1.087792	-0.677953	2.942891
C	2.256554	-1.523702	2.427588
C	2.232869	-3.006484	2.836969
C	1.694120	-3.974794	1.777648
C	0.231249	-3.811804	1.345319
C	-0.093388	-2.604584	0.458754
H	1.201223	0.383903	2.655717

H	1.116209	-0.678485	4.037176
H	2.368442	-1.451659	1.334239
H	3.172414	-1.051871	2.832871
H	3.262947	-3.319095	3.075483
H	1.663875	-3.125979	3.776616
H	1.828168	-5.001049	2.161950
H	2.336718	-3.904534	0.879509
H	-0.036744	-4.725308	0.779132
H	-0.422699	-3.840830	2.235965
H	0.652261	-2.516964	-0.347268
H	-1.070038	-2.785193	-0.023558
C	-1.940752	-1.241058	2.411336
C	-0.937977	-1.324659	3.402613
H	-2.336582	-2.158737	1.968658
H	-2.639176	-0.398964	2.454665
H	-0.942880	-0.582216	4.204087
H	-0.567559	-2.302207	3.717222

^{4}TS9-10B-10
Geometry with 85 atoms:
Total energy: -3274.477757980

Cr	-0.610043	-0.778723	0.884055
P	1.548225	-0.231848	-0.402921
P	-1.494043	0.572422	-0.998578
C	-0.357162	0.328140	-2.438493
C	1.096512	0.595823	-2.027577
H	-0.484441	-0.720706	-2.751994
H	-0.652138	0.968232	-3.285082
H	1.791539	0.244431	-2.800904
H	1.271645	1.675298	-1.920074
C	2.719119	-1.570869	-0.842739
C	2.494940	-2.893654	-0.435175
C	3.905839	-1.267290	-1.560866
C	3.410318	-3.907864	-0.730008
H	1.592064	-3.136294	0.124228
C	4.826373	-2.284161	-1.852547
C	4.571309	-3.595002	-1.438321
H	3.216344	-4.931865	-0.404776
H	5.740581	-2.062081	-2.402865
H	5.296519	-4.377610	-1.675062
C	2.599494	0.968121	0.517204
C	3.519983	0.464046	1.454127
C	2.447773	2.357898	0.398781
C	4.273199	1.332310	2.247913
H	3.660126	-0.614623	1.558367
C	3.205008	3.224976	1.192787
H	1.734589	2.786752	-0.305565
C	4.118939	2.716962	2.120340
H	4.988296	0.923444	2.966146
H	3.075479	4.304634	1.081933
H	4.711584	3.395745	2.738445
C	-1.332301	2.330316	-0.532244
C	-1.690473	3.365458	-1.410387
C	-0.830302	2.652778	0.747274
C	-1.549524	4.702742	-1.041872
H	-2.095164	3.111362	-2.393769
C	-0.691856	3.997523	1.122358
C	-1.049054	5.008459	0.226749
H	-1.831144	5.498689	-1.734103
H	-0.298136	4.270827	2.099565
H	-0.933636	6.050992	0.533099
C	-3.200601	0.360718	-1.600235
C	-4.254097	0.841875	-0.799471
C	-3.498322	-0.384429	-2.753908
C	-5.579924	0.589040	-1.154519
H	-4.037845	1.421063	0.102103
C	-4.829223	-0.634260	-3.103297
H	-2.701638	-0.776576	-3.388814
C	-5.870321	-0.150839	-2.306325
H	-6.390386	0.971386	-0.529185
H	-5.051093	-1.210449	-4.004873
H	-6.908821	-0.349065	-2.582251
O	4.070814	0.024434	-1.921163
O	-0.480142	1.612163	1.580699
C	5.292036	0.455957	-2.500581
H	5.463830	-0.010394	-3.486071
H	5.202258	1.542766	-2.629539
H	6.148969	0.241647	-1.839286
C	-0.005785	1.939708	2.892389
H	0.210669	0.996677	3.401362
H	0.920085	2.530577	2.836426
H	-0.776478	2.485980	3.458800
C	-2.439878	-0.897359	2.083826
C	-3.381108	-1.842415	2.818771
C	-3.309627	-3.340215	2.461398
C	-3.077944	-3.718699	0.988019
C	-1.614851	-3.725565	0.480303
C	-1.120921	-2.458857	-0.228072
H	-2.506121	0.125330	2.488224
H	-2.770845	-0.865051	1.030112
H	-3.254328	-1.734086	3.910571
H	-4.408274	-1.486141	2.612950
H	-2.533986	-3.842013	3.066323
H	-4.257399	-3.793795	2.796054
H	-3.696664	-3.082522	0.328394
H	-3.473301	-4.739687	0.860019
H	-0.940369	-4.006627	1.311008
H	-1.526894	-4.558912	-0.242701
H	-0.215538	-2.685261	-0.815944
H	-1.891250	-2.157530	-0.961711
C	0.654354	-1.502735	2.472814
C	-0.593608	-1.611192	3.104163
H	1.330222	-0.680400	2.727566
H	1.140537	-2.411208	2.107584
H	-1.026101	-2.602614	3.219251
H	-0.880320	-0.907009	3.889424

^{4}TS9-10B-11
Geometry with 85 atoms:
Total energy: -3274.478784290

Cr	-0.280628	-0.415462	1.188276
P	1.683206	0.000452	-0.426701
P	-1.436294	0.493071	-0.853349
C	-0.430169	0.062592	-2.347231
C	1.034217	0.456581	-2.130622
H	-0.521964	-1.024053	-2.482809
H	-0.841017	0.556093	-3.242335
H	1.677275	0.019852	-2.905993
H	1.138547	1.551202	-2.181791
C	2.758092	-1.485749	-0.560317
C	3.817852	-1.608166	0.354488
C	2.502756	-2.559352	-1.445227
C	4.614472	-2.753630	0.398936
H	4.028001	-0.787458	1.043626
C	3.304084	-3.710360	-1.402262
C	4.351869	-3.802826	-0.483103
H	5.433642	-2.821806	1.117720
H	3.115261	-4.540579	-2.081992
H	4.965409	-4.706851	-0.462654
C	2.897598	1.348320	-0.131656
C	4.013328	1.500185	-0.975574
C	2.692495	2.270110	0.904000
C	4.900912	2.559555	-0.782610
H	4.195728	0.782391	-1.779258
C	3.583649	3.331119	1.096251
H	1.831462	2.155741	1.559527
C	4.687456	3.477563	0.253260
H	5.765617	2.668760	-1.441824
H	3.414948	4.042843	1.908400
H	5.386040	4.304526	0.402721
C	-1.243935	2.309203	-0.702995
C	-1.485952	3.166202	-1.788009
C	-0.812403	2.859940	0.520066
C	-1.297545	4.543150	-1.673836
H	-1.831596	2.743119	-2.734842
C	-0.622112	4.242977	0.641194
C	-0.862515	5.073101	-0.456320
H	-1.489532	5.197811	-2.526338
H	-0.279471	4.684216	1.575869
H	-0.705745	6.149315	-0.351449
C	-3.187870	0.227514	-1.287387
C	-4.166432	0.799914	-0.453667
C	-3.584116	-0.614900	-2.339297
C	-5.519421	0.540040	-0.676756
H	-3.868447	1.457645	0.367792
C	-4.941133	-0.871776	-2.556786
H	-2.842662	-1.079959	-2.992166
C	-5.909176	-0.297443	-1.728043
H	-6.273224	0.993018	-0.028147
H	-5.242002	-1.524645	-3.379829
H	-6.968575	-0.501472	-1.901263
O	1.463071	-2.409332	-2.306475
O	-0.585213	1.988869	1.570201
C	1.089371	-3.478165	-3.160703
H	0.211854	-3.131785	-3.723663
H	1.892462	-3.728776	-3.874992
H	0.814084	-4.378645	-2.585243
C	-0.500510	2.542553	2.889104
H	-0.470064	1.700873	3.586768
H	0.413080	3.143913	3.017217
H	-1.385414	3.160927	3.105347
C	-1.951387	-0.682857	2.631759
C	-2.629764	-1.857302	3.337585
C	-2.237256	-3.279737	2.909403
C	-2.550862	-3.716024	1.473591
C	-1.969388	-2.862889	0.330349
C	-0.523189	-2.362873	0.506049
H	-2.169859	0.260968	3.151716
H	-2.378807	-0.575554	1.617535
H	-2.446608	-1.768796	4.423224
H	-3.724154	-1.739112	3.219578
H	-1.161686	-3.433992	3.092411
H	-2.744931	-3.982623	3.592065
H	-3.645818	-3.777395	1.340083
H	-2.177596	-4.750231	1.366894
H	-2.041790	-3.465047	-0.594868
H	-2.652577	-2.017213	0.146162
H	0.059938	-3.006835	1.188563
H	-0.002010	-2.390588	-0.461767
C	1.194198	-0.613827	2.727954
C	0.053006	-0.946203	3.482648
H	1.685418	0.351306	2.892237
H	1.846356	-1.420296	2.379564
H	-0.133372	-1.999133	3.687621
H	-0.289006	-0.278968	4.277489

^{4}TS9-10B-12
Geometry with 85 atoms:
Total energy: -3274.479133530

Cr	-0.078596	0.065277	1.162777
P	1.704219	0.124011	-0.711377
P	-1.571348	0.133684	-0.909151
C	-0.507906	-0.011732	-2.425646
C	0.786550	0.776151	-2.192467
H	-0.292760	-1.078915	-2.590169
H	-1.054885	0.365760	-3.303558
H	1.424139	0.790117	-3.088373
H	0.542949	1.824327	-1.966023
C	2.445460	-1.453518	-1.319654
C	2.466588	-1.784411	-2.684456
C	2.955121	-2.397981	-0.394788
C	2.951253	-3.015549	-3.131756
H	2.097128	-1.076426	-3.426862
C	3.430324	-3.640177	-0.840930
C	3.425098	-3.943152	-2.203761
H	2.955283	-3.244399	-4.199416
H	3.814908	-4.371230	-0.130803
H	3.802186	-4.913034	-2.537198
C	3.104394	1.297385	-0.486954
C	3.094375	2.588539	-1.043727
C	4.182321	0.921767	0.337553
C	4.138710	3.481485	-0.782074
H	2.279178	2.916908	-1.689978
C	5.223480	1.816635	0.591923
H	4.205548	-0.073412	0.782869
C	5.204924	3.100067	0.035956
H	4.118626	4.479152	-1.227985
H	6.055515	1.507530	1.229505
H	6.020851	3.798564	0.236803
C	-2.136715	1.881671	-0.964914
C	-3.233265	2.292520	-1.738487
C	-1.448940	2.844197	-0.194604
C	-3.658356	3.621865	-1.739934
H	-3.769341	1.554173	-2.338910
C	-1.880645	4.176679	-0.181169
C	-2.983024	4.555833	-0.952666
H	-4.515113	3.922850	-2.346285
H	-1.374437	4.927124	0.423731
H	-3.311693	5.597559	-0.931769
C	-3.077330	-0.854526	-1.205700
C	-4.232266	-0.578399	-0.449315
C	-3.083898	-1.946203	-2.090282
C	-5.368269	-1.378462	-0.578424

H	-4.250173	0.270240	0.238789
C	-4.224993	-2.744500	-2.214814
H	-2.203089	-2.190798	-2.686634
C	-5.366704	-2.465310	-1.459079
H	-6.258505	-1.151889	0.013208
H	-4.218724	-3.589344	-2.907724
H	-6.256303	-3.091894	-1.557733
O	2.970416	-2.025484	0.908960
O	-0.340857	2.416460	0.513979
C	3.277098	-2.978852	1.915864
H	3.146302	-2.466521	2.878058
H	2.593177	-3.842733	1.871680
H	4.321225	-3.326579	1.839958
C	0.471393	3.409447	1.153869
H	0.740728	4.207067	0.446442
H	-0.045637	3.838762	2.026800
H	1.388919	2.908359	1.471497
C	-1.604126	0.527064	2.692454
C	-2.286306	-0.235285	3.819389
C	-2.237231	-1.770018	3.713502
C	-2.659323	-2.314960	2.333342
C	-1.516903	-2.774001	1.401557
C	-0.206542	-1.978670	1.392158
H	-1.708182	1.615449	2.810150
H	-2.125124	0.267485	1.749822
H	-1.884732	0.082911	4.797772
H	-3.349946	0.072742	3.830863
H	-1.228484	-2.136881	3.968658
H	-2.898581	-2.176037	4.496043
H	-3.267082	-1.552625	1.818970
H	-3.342644	-3.169636	2.464683
H	-1.262085	-3.818397	1.672317
H	-1.922145	-2.837350	0.377941
H	0.348920	-2.144834	2.331625
H	0.436141	-2.368484	0.584987
C	1.525042	0.411923	2.562497
C	0.450252	0.452209	3.462123
H	2.065003	1.328419	2.313390
H	2.102979	-0.504165	2.445505
H	0.223724	-0.439808	4.047428
H	0.195171	1.391650	3.958179

^{4}TS9-10B-13
Geometry with 85 atoms:
Total energy: -3274.478153470

Cr	-0.174324	-0.488551	0.994619
P	1.620383	0.075057	-0.765205
P	-1.634667	0.439677	-0.874149
C	-0.543659	0.967445	-2.291498
C	0.692968	0.066176	-2.388536
H	-1.117156	0.973466	-3.231037
H	-0.255125	2.009689	-2.086375
H	0.390609	-0.970988	-2.598877
H	1.363314	0.394581	-3.197903
C	2.944186	-1.170805	-0.971286
C	2.949527	-2.125074	-1.998271
C	3.969654	-1.216549	0.006224
C	3.939349	-3.110666	-2.062506
H	2.174771	-2.111793	-2.765635
C	4.963174	-2.202524	-0.057617
C	4.939133	-3.145559	-1.090077
H	3.924997	-3.845421	-2.870051
H	5.754014	-2.241497	0.691046
H	5.716543	-3.912579	-1.129487
C	2.458068	1.711571	-0.831302
C	3.715635	1.876782	-1.435305
C	1.799459	2.833218	-0.303085
C	4.300726	3.142880	-1.504648
H	4.243537	1.014243	-1.848711
C	2.384461	4.101161	-0.381223
H	0.826614	2.716960	0.172786
C	3.637648	4.257700	-0.978733
H	5.281395	3.260208	-1.972681
H	1.858970	4.967219	0.029290
H	4.099105	5.246626	-1.035489
C	-2.426287	1.967931	-0.257588
C	-3.505438	2.572345	-0.920831
C	-1.942297	2.548272	0.935217
C	-4.107039	3.725313	-0.415021
H	-3.885861	2.120351	-1.839898
C	-2.552652	3.698418	1.452872
C	-3.629212	4.277668	0.774771
H	-4.945642	4.184291	-0.942484
H	-2.206540	4.150945	2.380554
H	-4.096948	5.173126	1.191038
C	-2.987671	-0.557443	-1.585086
C	-4.188904	-0.703523	-0.865753
C	-2.791978	-1.311942	-2.753689
C	-5.177071	-1.579952	-1.317647
H	-4.357178	-0.127000	0.046893
C	-3.784363	-2.189249	-3.199977
H	-1.862620	-1.231311	-3.321641
C	-4.976912	-2.326177	-2.484017
H	-6.108360	-1.681197	-0.755149
H	-3.622130	-2.768933	-4.111899
H	-5.750589	-3.013247	-2.834838
O	3.913545	-0.255253	0.956741
O	-0.857733	1.946151	1.540552
C	4.872955	-0.220388	1.999185
H	5.892618	-0.069481	1.604983
H	4.608163	0.634915	2.634681
H	4.847487	-1.142143	2.606204
C	-0.265819	2.609047	2.662399
H	0.659929	2.075174	2.897326
H	-0.012567	3.651742	2.415210
H	-0.939024	2.587335	3.533893
C	-1.796862	-0.928637	2.465277
C	-2.242180	-2.192059	3.201399
C	-1.538257	-3.507219	2.832785
C	-1.808790	-4.092024	1.442163
C	-1.511595	-3.193971	0.230072
C	-0.175508	-2.434849	0.256025
H	-2.174326	-0.020954	2.956478
H	-2.232621	-0.930530	1.448969
H	-2.116934	-2.028152	4.286216
H	-3.332288	-2.317511	3.053855
H	-0.449211	-3.385224	2.957708
H	-1.831239	-4.266300	3.578268
H	-2.863383	-4.416261	1.382604
H	-1.205796	-5.013683	1.355421
H	-1.548782	-3.835843	-0.669340
H	-2.351721	-2.496408	0.089185
H	0.590601	-2.975012	0.841265
H	0.227090	-2.362704	-0.768474
C	1.334954	-0.553502	2.508938
C	0.222614	-0.744055	3.344023
H	1.830326	0.419879	2.451701
H	1.970728	-1.406805	2.259672
H	0.072383	-1.719567	3.802667
H	-0.147717	0.088253	3.947245

^{4}TS9-10B-14
Geometry with 85 atoms:
Total energy: -3274.478845890

Cr	-0.238141	-0.643622	0.939364
P	1.611787	-0.006319	-0.752088
P	-1.590774	0.514081	-0.845908
C	-0.522366	0.870820	-2.338391
C	0.697554	-0.061157	-2.379838
H	-1.122638	0.782935	-3.256430
H	-0.207493	1.922710	-2.257930
H	0.378372	-1.102776	-2.538964
H	1.376477	0.217491	-3.200719
C	2.962969	-1.227058	-0.925064
C	3.024109	-2.176760	-1.954550
C	3.952550	-1.255026	0.089224
C	4.035431	-3.142327	-1.984678
H	2.277394	-2.175720	-2.749546
C	4.965766	-2.222399	0.060794
C	4.998083	-3.161837	-0.974908
H	4.066020	-3.874199	-2.794404
H	5.728466	-2.249928	0.838766
H	5.790671	-3.914109	-0.987242
C	2.442504	1.633640	-0.836200
C	1.816741	2.752565	-0.267085
C	3.671878	1.800275	-1.496635
C	2.401711	4.019289	-0.360306
H	0.868482	2.634841	0.250477
C	4.258249	3.064871	-1.581935
H	4.178473	0.940463	-1.941250
C	3.625584	4.177359	-1.015130
H	1.897797	4.881778	0.083294
H	5.216176	3.182652	-2.094807
H	4.087763	5.165106	-1.085246
C	-2.062117	2.134174	-0.146708
C	-2.947440	3.005359	-0.800744
C	-1.522681	2.516545	1.101615
C	-3.304292	4.229004	-0.233748
H	-3.370774	2.709062	-1.763705
C	-1.887390	3.739386	1.679557
C	-2.775446	4.585116	1.008773
H	-3.993952	4.896320	-0.754486
H	-1.490759	4.044680	2.646094
H	-3.052792	5.535362	1.471296
C	-3.135507	-0.245674	-1.446741
C	-4.349218	-0.036918	-0.766801
C	-3.085573	-1.187159	-2.490023
C	-5.492376	-0.749732	-1.135662
H	-4.406282	0.683196	0.052024
C	-4.232128	-1.898714	-2.851874
H	-2.151191	-1.378052	-3.023593
C	-5.436936	-1.682601	-2.175806
H	-6.431375	-0.575733	-0.604604
H	-4.182456	-2.626199	-3.665676
H	-6.332224	-2.240602	-2.460195
O	3.843174	-0.295986	1.037824
O	-0.614031	1.660228	1.695976
C	4.777310	-0.233714	2.101587
H	4.487343	0.627981	2.717651
H	4.748256	-1.147233	2.720789
H	5.804015	-0.074008	1.729559
C	0.041019	2.092223	2.894912
H	0.803800	1.342235	3.125116
H	0.539573	3.061702	2.741090
H	-0.673449	2.163455	3.729633
C	-1.906964	-0.975933	2.435557
C	-2.760444	-2.232903	2.576747
C	-3.080389	-2.976168	1.266970
C	-2.121508	-4.102656	0.868261
C	-0.632770	-3.743685	0.782351
C	-0.304377	-2.489696	-0.036377
H	-2.013447	-0.320229	3.308078
H	-2.305949	-0.380939	1.591080
H	-2.318126	-2.930976	3.311999
H	-3.715408	-1.914903	3.034315
H	-4.090279	-3.412163	1.345570
H	-3.145792	-2.241863	0.448274
H	-2.448320	-4.485770	-0.115352
H	-2.239434	-4.944913	1.573857
H	-0.208386	-3.674387	1.798336
H	-0.112152	-4.611778	0.334912
H	0.712938	-2.593705	-0.447316
H	-0.992836	-2.414802	-0.898059
C	1.214909	-1.224001	2.384313
C	0.075644	-1.423953	3.189244
H	1.863487	-0.364182	2.571683
H	1.710370	-2.082639	1.921812
H	-0.274222	-2.437255	3.390699
H	-0.101634	-0.729681	4.013698

^{4}TS9-10B-15
Geometry with 85 atoms:
Total energy: -3274.478913310

Cr	0.155815	-0.748822	1.062071
P	-1.673557	0.590658	-0.493210
P	1.607880	0.501467	-0.595289
C	0.642523	1.415730	-1.903059
C	-0.744128	0.795752	-2.101573
H	0.559058	2.458180	-1.570574
H	1.204709	1.399434	-2.849273
H	-1.342866	1.397688	-2.802113
H	-0.641581	-0.213571	-2.526934
C	-2.402914	2.267680	-0.197114
C	-3.750485	2.546787	-0.476767
C	-1.596764	3.313575	0.318203
C	-4.299053	3.810510	-0.242180
H	-4.390706	1.764156	-0.886049
C	-2.146094	4.580557	0.557205
C	-3.493980	4.822793	0.278922
H	-5.350739	3.997580	-0.469121
H	-1.528163	5.383728	0.956935
H	-3.909103	5.815445	0.469785
C	-3.135146	-0.427552	-0.950099

C -4.053640 -0.748715 0.068965
C -3.351983 -0.946308 -2.238011
C -5.150426 -1.572059 -0.190091
H -3.923496 -0.334805 1.072064
C -4.447522 -1.778466 -2.493553
H -2.675545 -0.708797 -3.059932
C -5.345896 -2.097055 -1.472357
H -5.854073 -1.805508 0.612631
H -4.600446 -2.173095 -3.501145
H -6.200932 -2.746282 -1.675597
C 2.321402 -0.907788 -1.531789
C 3.592895 -0.889515 -2.118193
C 1.538423 -2.075397 -1.633471
C 4.076249 -2.002513 -2.811893
H 4.212194 0.005846 -2.026035
C 2.011396 -3.189606 -2.332456
C 3.281069 -3.144045 -2.919436
H 5.070030 -1.976363 -3.263688
H 1.416596 -4.098295 -2.413893
H 3.647997 -4.020759 -3.458341
C 3.015467 1.587788 -0.177028
C 3.701404 1.362340 1.030448
C 3.415042 2.651900 -1.004513
C 4.767292 2.185679 1.400674
H 3.404081 0.540734 1.684755
C 4.478090 3.477064 -0.626121
H 2.903952 2.846818 -1.948981
C 5.154813 3.246592 0.575491
H 5.293677 2.000063 2.340029
H 4.780003 4.302201 -1.275875
H 5.985512 3.893226 0.868525
O -0.287080 3.020437 0.545060
O 0.306222 -2.054380 -0.999317
C 0.590123 4.010954 1.066337
H 0.241700 4.385172 2.043578
H 1.563806 3.522402 1.194757
H 0.701032 4.856757 0.366791
C -0.636558 -3.080255 -1.335016
H -1.586505 -2.808360 -0.862709
H -0.780189 -3.125925 -2.425330
H -0.307044 -4.059681 -0.957599
C -1.335245 -1.925542 2.084921
C -1.335138 -2.970188 3.192820
C -0.018076 -3.728527 3.425901
C 0.636359 -4.247025 2.130104
C 1.810855 -3.403395 1.584041
C 1.764231 -1.878679 1.760037
H -2.333474 -1.486689 1.973228
H -1.113720 -2.435682 1.122330
H -1.678630 -2.517352 4.139480
H -2.115531 -3.713193 2.935077
H 0.694824 -3.093604 3.977870
H -0.237303 -4.572497 4.099800
H -0.148022 -4.350188 1.359183
H 1.008640 -5.272177 2.288099
H 2.733552 -3.759606 2.083230
H 1.957145 -3.655481 0.519818
H 1.840308 -1.622072 2.830474
H 2.672473 -1.465348 1.288077
C 0.341495 0.721058 2.630107
C -0.519300 -0.162483 3.276364
H -0.053305 1.632599 2.182681
H 1.407856 0.714147 2.868499
H -0.122140 -0.862580 4.012482
H -1.573860 0.093242 3.399937

4TS9-10B-16
Geometry with 85 atoms:
Total energy: -3274.479190040
Cr -0.231214 -0.930370 0.870846
P 1.534385 -0.158861 -0.812448
P -1.564715 0.485013 -0.766507
C -0.618614 0.720662 -2.363981
C 0.602991 -0.205682 -2.422774
H -1.282833 0.546265 -3.222077
H -0.309184 1.775425 -2.406579
H 0.282282 -1.247408 -2.569365
H 1.253975 0.057842 -3.269739
C 2.975747 -1.256827 -1.075272
C 3.093324 -2.128705 -2.166694
C 3.984196 -1.266822 -0.080379
C 4.186610 -2.993452 -2.281018
H 2.329631 -2.144684 -2.945319
C 5.081608 -2.130064 -0.195516
C 5.174402 -2.988643 -1.295643
H 4.261709 -3.666200 -3.137780
H 5.862832 -2.139697 0.564522
H 6.032486 -3.660450 -1.376092
C 2.212101 1.552716 -0.764860
C 2.280649 2.224168 0.465116
C 2.660366 2.205959 -1.924899
C 2.772397 3.529042 0.535733
H 1.954261 1.713693 1.370246
C 3.150260 3.512976 -1.853995
H 2.640960 1.698928 -2.891944
C 3.203466 4.178211 -0.625085
H 2.816638 4.042909 1.499246
H 3.494591 4.012428 -2.762984
H 3.584497 5.201065 -0.572394
C -1.549800 2.144992 0.009748
C -2.080548 3.258426 -0.661757
C -0.977348 2.325003 1.284238
C -2.040460 4.530871 -0.094590
H -2.538446 3.116858 -1.644435
C -0.935182 3.603005 1.859434
C -1.463200 4.694681 1.166767
H -2.456438 5.386424 -0.630397
H -0.488440 3.765347 2.838639
H -1.419657 5.685012 1.626152
C -3.320830 0.194202 -1.187685
C -3.702334 -0.482969 -2.358032
C -4.303571 0.525122 -0.235845
C -5.042597 -0.814303 -2.575110
H -2.961806 -0.768206 -3.108379
C -5.640654 0.189844 -0.457385
H -4.027138 1.053715 0.679768
C -6.013720 -0.481462 -1.626392
H -5.326951 -1.338398 -3.490773
H -6.395047 0.456421 0.286775
H -7.060394 -0.743763 -1.798030
O 3.798918 -0.404356 0.947286
O -0.464539 1.212147 1.928187
C 4.731066 -0.349836 2.011617
H 4.367054 0.421716 2.703507
H 4.792883 -1.313835 2.545986
H 5.735636 -0.061071 1.658149
C -0.077751 1.365117 3.299040
H 0.800220 2.023806 3.391050
H -0.911095 1.767069 3.895342
H 0.180250 0.372849 3.676339
C -1.851611 -1.476038 2.279011
C -2.651806 -2.740946 2.557092
C -2.679666 -3.801574 1.439863
C -2.918991 -3.235897 0.023535
C -1.662776 -3.147667 -0.869091
C -0.356476 -2.700089 -0.208584
H -1.924237 -0.766551 3.114656
H -2.310883 -0.965631 1.410248
H -2.314193 -3.208572 3.499252
H -3.694964 -2.424036 2.751944
H -1.744183 -4.385709 1.452188
H -3.472658 -4.523290 1.693798
H -3.392389 -2.243628 0.101431
H -3.660136 -3.857368 -0.504527
H -1.490003 -4.151711 -1.306312
H -1.897229 -2.499267 -1.731810
H -0.041064 -3.454262 0.530678
H 0.447648 -2.701731 -0.965257
C 1.293085 -1.662432 2.204484
C 0.170797 -2.177907 2.870769
H 1.836246 -0.808603 2.619048
H 1.881871 -2.313434 1.553238
H -0.109500 -3.219073 2.704568
H -0.108528 -1.799014 3.856515

4TS9-10B-17
Geometry with 85 atoms:
Total energy: -3274.480642400
Cr -0.209387 0.052938 1.275803
P -1.779014 0.099433 -0.672413
P 1.514334 0.081227 -0.820724
C 0.441353 0.571606 -2.273447
C -0.906046 -0.157650 -2.291370
H 0.267540 1.653892 -2.178643
H 0.993366 0.404090 -3.210555
H -1.542132 0.212810 -3.110491
H -0.753239 -1.235111 -2.422513
C -2.346050 1.840697 -0.789212
C -3.528194 2.201864 -1.451656
C -1.553048 2.852030 -0.202642
C -3.931615 3.536145 -1.530524
H -4.147092 1.422315 -1.901958
C -1.955850 4.191871 -0.278335
C -3.141778 4.523968 -0.940742
H -4.856942 3.799962 -2.046758
H -1.362274 4.984367 0.174094
H -3.445742 5.572341 -0.989410
C -3.290232 -0.923747 -0.719659
C -3.435975 -2.010329 -1.598861
C -4.301888 -0.667846 0.225679
C -4.572946 -2.822879 -1.532166
H -2.672060 -2.235111 -2.344514
C -5.435053 -1.479766 0.285293
H -4.208555 0.177983 0.909855
C -5.572042 -2.561953 -0.591470
H -4.676637 -3.661968 -2.224530
H -6.215066 -1.266638 1.020194
H -6.458910 -3.198338 -0.542658
C 2.513389 -1.345190 -1.432410
C 3.873470 -1.228713 -1.758000
C 1.898183 -2.615338 -1.553643
C 4.617312 -2.336184 -2.175137
H 4.366901 -0.258786 -1.682545
C 2.644037 -3.728638 -1.963102
C 4.000006 -3.583481 -2.270097
H 5.674424 -2.219265 -2.422884
H 2.173810 -4.707621 -2.051182
H 4.571394 -4.458056 -2.590816
C 2.742764 1.442443 -0.683005
C 2.754956 2.577393 -1.510834
C 3.679135 1.362908 0.366715
C 3.667668 3.612815 -1.282338
H 2.058337 2.671396 -2.344966
C 4.592671 2.394882 0.589264
H 3.707078 0.479089 1.007341
C 4.584049 3.528456 -0.230771
H 3.664298 4.487751 -1.937325
H 5.313756 2.312544 1.406290
H 5.295252 4.339191 -0.055214
O -0.392356 2.456987 0.430541
O 0.570568 -2.667657 -1.272173
C 0.456477 3.475968 0.971464
H 1.351918 2.977770 1.354204
H 0.763232 4.185472 0.188921
H -0.046582 4.012144 1.792354
C -0.105024 -3.915671 -1.231920
H -1.130423 -3.700146 -0.906831
H -0.130348 -4.392497 -2.226999
H 0.360925 -4.603394 -0.506520
C 1.279761 0.557043 2.824832
C 2.119416 -0.713868 2.987384
C 1.688061 -1.660193 4.122989
C 0.816049 -2.850514 3.706587
C -0.539087 -2.548066 3.055754
C -0.487662 -1.955370 1.645914
H 1.679293 1.192307 2.015980
H 1.395100 1.160475 3.731302
H 2.195269 -1.281169 2.044473
H 3.149792 -0.365620 3.195197
H 2.594350 -2.069176 4.599708
H 1.180207 -1.079429 4.913666
H 0.642619 -3.470967 4.603130
H 1.399605 -3.484238 3.012130
H -1.086467 -3.509184 3.001260
H -1.149526 -1.925482 3.735141
H 0.314264 -2.426972 1.056581
H -1.438309 -2.157833 1.125074
C -1.842994 0.600508 2.522770
C -0.797368 0.855624 3.434056
H -2.455196 -0.296153 2.649866
H -2.344974 1.458858 2.065635
H -0.544271 1.897702 3.645563
H -0.633599 0.180681 4.276036

^{4}TS9-10B-18
Geometry with 85 atoms:
Total energy: -3274.479317090

Cr	0.190397	-0.735528	1.047058
P	1.616639	0.511755	-0.634086
P	-1.673444	0.649361	-0.493104
C	-0.741777	0.904841	-2.092792
C	0.652846	1.501176	-1.881731
H	-0.653584	-0.090475	-2.554164
H	-1.334190	1.538012	-2.770900
H	1.204945	1.521769	-2.833953
H	0.585463	2.527997	-1.500505
C	2.253858	-0.895766	-1.630377
C	3.494264	-0.888591	-2.279925
C	1.458779	-2.059245	-1.688152
C	3.937708	-2.010385	-2.986172
H	4.122185	0.004089	-2.224581
C	1.895658	-3.185365	-2.390488
C	3.136541	-3.151788	-3.037140
H	4.907016	-1.992570	-3.488697
H	1.294405	-4.092845	-2.431922
H	3.475966	-4.037183	-3.579920
C	3.074382	1.527169	-0.211261
C	3.458443	2.647947	-0.967514
C	3.815252	1.184501	0.935007
C	4.561181	3.414645	-0.578919
H	2.905170	2.933509	-1.863922
C	4.919150	1.950740	1.315430
H	3.530652	0.315641	1.531549
C	5.291561	3.069212	0.561999
H	4.850971	4.284911	-1.172949
H	5.487805	1.675223	2.206869
H	6.152374	3.670910	0.863741
C	-2.386938	2.316010	-0.126578
C	-3.732714	2.623616	-0.380497
C	-1.562321	3.323588	0.433091
C	-4.262010	3.881667	-0.079079
H	-4.385060	1.868401	-0.821453
C	-2.091825	4.584005	0.739775
C	-3.439007	4.856258	0.484629
H	-5.312820	4.093969	-0.287181
H	-1.459821	5.357560	1.174536
H	-3.839937	5.843316	0.727789
C	-3.137844	-0.340358	-1.002174
C	-4.041365	-0.737065	0.003250
C	-3.368920	-0.770839	-2.320281
C	-5.136456	-1.548670	-0.297491
H	-3.900170	-0.392429	1.030168
C	-4.462863	-1.590631	-2.618283
H	-2.706211	-0.472187	-3.133612
C	-5.345869	-1.985296	-1.610159
H	-5.828092	-1.841363	0.496221
H	-4.627036	-1.915769	-3.648696
H	-6.199394	-2.625146	-1.846930
O	0.250501	-2.021223	-1.009338
O	-0.256583	2.997160	0.632101
C	-0.730702	-3.017676	-1.326235
H	-0.886298	-3.068206	-2.414462
H	-0.433722	-4.005105	-0.941326
H	-1.666458	-2.707306	-0.849088
C	0.646318	3.946171	1.182885
H	0.758308	4.824103	0.523909
H	0.324619	4.278048	2.184476
H	1.613719	3.435647	1.266794
C	-1.348319	-1.839545	2.113926
C	-1.460707	-2.958956	3.141259
C	-0.592663	-4.196396	2.891485
C	0.934150	-4.036044	2.946394
C	1.637737	-3.444176	1.709331
C	1.797955	-1.920642	1.642953
H	-2.269981	-1.249120	2.071339
H	-1.231147	-2.310057	1.113217
H	-1.274821	-2.579492	4.162226
H	-2.514457	-3.293775	3.155737
H	-0.882374	-4.949537	3.644115
H	-0.868312	-4.637290	1.914427
H	1.350736	-5.044642	3.107470
H	1.217313	-3.457619	3.845577
H	2.652745	-3.883988	1.675209
H	1.144251	-3.826875	0.796423
H	2.163503	-1.548412	2.616930
H	2.592804	-1.695523	0.912373
C	0.454196	0.651892	2.645566
C	-0.276744	-0.325716	3.330780
H	-0.041661	1.575747	2.346446
H	1.540243	0.696778	2.758734
H	0.253202	-1.077208	3.918095
H	-1.287247	-0.104789	3.681181

^{4}TS9-10B-19
Geometry with 85 atoms:
Total energy: -3274.477985440

Cr	-0.244308	-0.649755	1.003502
P	1.673494	0.061423	-0.629370
P	-1.546652	0.296272	-0.911894
C	-0.529211	0.085685	-2.445720
C	0.877299	0.658736	-2.228703
H	-0.489691	-0.996025	-2.654085
H	-1.017953	0.573525	-3.303818
H	1.528440	0.388616	-3.071558
H	0.826615	1.756096	-2.203567
C	3.100970	-0.939980	-1.237888
C	3.984351	-0.332852	-2.148974
C	3.363125	-2.265372	-0.821048
C	5.085039	-1.013670	-2.665784
H	3.810605	0.702920	-2.452585
C	4.471465	-2.954631	-1.347308
C	5.319030	-2.331240	-2.262440
H	5.755075	-0.519405	-3.372118
H	4.679295	-3.978372	-1.037936
H	6.176023	-2.882857	-2.656926
C	2.545998	1.529622	0.072292
C	2.179279	2.859090	-0.184712
C	3.577625	1.278586	0.997747
C	2.828929	3.913701	0.466975
H	1.379392	3.096733	-0.886027
C	4.221352	2.331641	1.649145
H	3.887365	0.250780	1.202468
C	3.848152	3.655154	1.386533
H	2.531205	4.942608	0.249967
H	5.023199	2.117877	2.360194
H	4.355630	4.480035	1.892488
C	-1.561474	2.105677	-0.622377
C	-2.148186	2.984809	-1.547008
C	-0.977972	2.630446	0.549662
C	-2.156010	4.361667	-1.328770
H	-2.615053	2.574404	-2.446291
C	-0.990443	4.014916	0.776409
C	-1.575500	4.867466	-0.162282
H	-2.614786	5.033267	-2.057164
H	-0.537124	4.442222	1.668550
H	-1.574848	5.943509	0.027703
C	-3.273873	-0.097382	-1.351503
C	-4.296076	0.336899	-0.487009
C	-3.604671	-0.883672	-2.467037
C	-5.624405	-0.009689	-0.737381
H	-4.054797	0.954955	0.381750
C	-4.937284	-1.229602	-2.711438
H	-2.831188	-1.238361	-3.150855
C	-5.947494	-0.796496	-1.848485
H	-6.410850	0.335448	-0.061872
H	-5.184943	-1.840493	-3.582913
H	-6.987643	-1.069031	-2.042545
O	2.526389	-2.807534	0.090544
O	-0.395815	1.744217	1.430913
C	2.667064	-4.166767	0.471560
H	1.845955	-4.377454	1.168515
H	2.578760	-4.841916	-0.396630
H	3.627513	-4.349327	0.983467
C	0.119001	2.267301	2.662559
H	0.975379	2.932403	2.475762
H	-0.669028	2.799949	3.217239
H	0.453354	1.414053	3.257814
C	-1.831462	-0.758793	2.547501
C	-2.647121	-1.868458	3.194534
C	-2.722111	-3.190628	2.410903
C	-3.074873	-3.020988	0.917850
C	-1.899079	-3.184762	-0.065602
C	-0.546018	-2.570710	0.306865
H	-1.853256	0.165062	3.142355
H	-2.306301	-0.512073	1.579068
H	-2.286300	-2.065566	4.219662
H	-3.678825	-1.486246	3.320515
H	-1.770844	-3.740840	2.508406
H	-3.474573	-3.825688	2.905895
H	-3.546683	-2.036340	0.764394
H	-3.850786	-3.750263	0.633614
H	-1.737442	-4.270711	-0.220553
H	-2.226760	-2.806009	-1.048296
H	-0.077048	-3.151546	1.119134
H	0.141183	-2.660751	-0.550931
C	1.280208	-1.023099	2.481496
C	0.155891	-1.358469	3.252035
H	1.824043	-0.097178	2.690878
H	1.857416	-1.808186	1.990156
H	-0.127571	-2.409257	3.336189
H	-0.105067	-0.760161	4.128178

^{4}TS9-10B-20
Geometry with 85 atoms:
Total energy: -3274.476021460

Cr	-0.354701	-0.483848	1.105634
P	1.708735	-0.093707	-0.434797
P	-1.357224	0.579115	-0.934529
C	-0.349973	0.114227	-2.414171
C	1.129377	0.414049	-2.154932
H	-0.501559	-0.961676	-2.573285
H	-0.707339	0.648125	-3.308995
H	1.759436	-0.068415	-2.914069
H	1.302722	1.498957	-2.211334
C	2.806072	-1.556729	-0.621212
C	3.973045	-1.654909	0.152775
C	2.433616	-2.654759	-1.431618
C	4.761022	-2.808348	0.130400
H	4.272130	-0.816285	0.784893
C	3.222993	-3.813213	-1.453161
C	4.380644	-3.883990	-0.673281
H	5.666139	-2.862292	0.738850
H	2.942439	-4.661198	-2.077497
H	4.987280	-4.792507	-0.700207
C	2.902918	1.248187	-0.029231
C	3.796760	1.724522	-1.006678
C	2.951525	1.799064	1.259193
C	4.702038	2.742028	-0.701068
H	3.797718	1.295804	-2.011484
C	3.862115	2.815627	1.565803
H	2.281556	1.429774	2.032353
C	4.734698	3.292776	0.585271
H	5.389861	3.103548	-1.469413
H	3.890708	3.231942	2.576016
H	5.445237	4.088340	0.822490
C	-1.082131	2.378499	-0.750663
C	-1.353551	3.277649	-1.794597
C	-0.551059	2.872600	0.459248
C	-1.099338	4.641286	-1.654550
H	-1.777305	2.898135	-2.728222
C	-0.294446	4.243086	0.603970
C	-0.566491	5.114893	-0.452562
H	-1.316160	5.329256	-2.474216
H	0.124315	4.641278	1.526471
H	-0.357725	6.180124	-0.327446
C	-3.113347	0.370209	-1.374837
C	-3.527685	-0.546180	-2.356853
C	-4.082754	1.044755	-0.608585
C	-4.890072	-0.773812	-2.573667
H	-2.795554	-1.086812	-2.960307
C	-5.441143	0.812912	-0.830748
H	-3.775291	1.758898	0.160041
C	-5.847693	-0.097217	-1.812908
H	-5.203170	-1.482863	-3.343868
H	-6.186345	1.345530	-0.234815
H	-6.911440	-0.277695	-1.985554
O	1.297461	-2.508068	-2.160496
O	-0.300891	1.965784	1.469799
C	0.727787	-3.630881	-2.811924
H	-0.223021	-3.291713	-3.245395
H	1.373510	-4.001839	-3.626131
H	0.524631	-4.450079	-2.101354
C	-0.104608	2.477224	2.792706
H	-0.967995	3.085559	3.105996
H	-0.011211	1.611079	3.455215
H	0.815746	3.075685	2.860569

C	-2.151093	-0.441370	2.352303
C	-3.107640	-1.255653	3.210093
C	-3.162197	-2.777022	2.957511
C	-2.900995	-3.271654	1.522570
C	-1.416707	-3.492046	1.146477
C	-0.688849	-2.392633	0.368116
H	-2.182567	0.622161	2.634414
H	-2.507426	-0.522392	1.309303
H	-2.912366	-1.076276	4.282231
H	-4.115596	-0.836581	3.029651
H	-2.454477	-3.297458	3.626100
H	-4.157769	-3.123443	3.280439
H	-3.385321	-2.604473	0.786034
H	-3.417644	-4.239632	1.419331
H	-0.850216	-3.753453	2.058501
H	-1.365769	-4.407904	0.525709
H	0.335334	-2.737049	0.153620
H	-1.186410	-2.260395	-0.610416
C	0.948200	-1.029597	2.727895
C	-0.290339	-1.124648	3.381130
H	1.615601	-0.195744	2.963721
H	1.440194	-1.939842	2.371346
H	-0.725828	-2.109476	3.538293
H	-0.565657	-0.390788	4.143356

^{4}TS9-10B-21
Geometry with 85 atoms:
Total energy: -3274.478210080

Cr	-0.541991	-0.990647	0.973948
P	1.572922	-0.456933	-0.358463
P	-1.402062	0.463592	-0.906289
C	-0.275383	0.454969	-2.393839
C	1.039406	-0.300958	-2.136957
H	-0.807433	-0.006362	-3.237032
H	-0.095646	1.502795	-2.671842
H	0.927234	-1.353867	-2.440434
H	1.869565	0.114952	-2.724961
C	3.000145	-1.600822	-0.502283
C	2.924141	-2.906504	0.003785
C	4.187926	-1.194366	-1.166069
C	4.003039	-3.788750	-0.096448
H	2.002146	-3.245243	0.475037
C	5.279158	-2.072534	-1.246140
C	5.180710	-3.359624	-0.710268
H	3.921648	-4.800827	0.304954
H	6.200885	-1.763915	-1.739151
H	6.036858	-4.034705	-0.786942
C	2.290131	1.149898	0.161926
C	2.208985	2.316819	-0.611896
C	2.891538	1.210525	1.430088
C	2.714664	3.524223	-0.122628
H	1.758341	2.296523	-1.604576
C	3.408398	2.415612	1.912067
H	2.968965	0.306848	2.040852
C	3.315077	3.578024	1.138568
H	2.638424	4.427494	-0.732686
H	3.886221	2.446771	2.894637
H	3.713088	4.522693	1.517010
C	-1.219758	2.162666	-0.237033
C	-1.522279	3.279628	-1.032491
C	-0.752391	2.364293	1.076253
C	-1.355056	4.576532	-0.551018
H	-1.905852	3.123617	-2.044245
C	-0.580546	3.667957	1.564579
C	-0.879258	4.761082	0.749745
H	-1.597039	5.434578	-1.181453
H	-0.201768	3.847999	2.568342
H	-0.736915	5.769903	1.144428
C	-3.131813	0.415642	-1.502097
C	-4.132510	0.947765	-0.666357
C	-3.509871	-0.255808	-2.676419
C	-5.480525	0.807274	-1.000239
H	-3.859196	1.479832	0.247835
C	-4.861027	-0.389747	-3.008232
H	-2.760494	-0.688899	-3.341494
C	-5.848681	0.136245	-2.170885
H	-6.246507	1.226052	-0.343025
H	-5.140954	-0.912385	-3.926032
H	-6.904088	0.025500	-2.431000
O	4.180693	0.041769	-1.710824
O	-0.476669	1.249756	1.842393
C	5.368245	0.596040	-2.252270
H	5.118586	1.623675	-2.548539
H	6.178182	0.626034	-1.503389
H	5.710980	0.037538	-3.140578
C	-0.177391	1.463403	3.227889
H	0.787162	1.980123	3.342287
H	-0.980218	2.039961	3.711999
H	-0.116013	0.481378	3.701498
C	-2.411024	-1.126721	2.137992
C	-3.423322	-2.228048	2.417092
C	-3.455814	-3.391747	1.409466
C	-3.455880	-2.948992	-0.069000
C	-2.111787	-3.105107	-0.810696
C	-0.818291	-2.762969	-0.060450
H	-2.465511	-0.325874	2.888813
H	-2.676485	-0.656749	1.172720
H	-3.287186	-2.628093	3.437653
H	-4.424961	-1.755484	2.425073
H	-2.608624	-4.074222	1.592820
H	-4.357256	-3.988310	1.623555
H	-3.796045	-1.902641	-0.135694
H	-4.211324	-3.523691	-0.628913
H	-2.031340	-4.158622	-1.145619
H	-2.167324	-2.515888	-1.742302
H	-0.620207	-3.522705	0.716346
H	0.021402	-2.845189	-0.772927
C	0.654368	-1.816112	2.597813
C	-0.624416	-2.078571	3.102494
H	1.262893	-1.016364	3.030912
H	1.217655	-2.629785	2.141387
H	-1.046471	-3.075382	2.968323
H	-0.996127	-1.552933	3.984067

^{4}TS9-10B-22
Geometry with 85 atoms:
Total energy: -3274.479280310

Cr	-0.205966	-0.922939	0.899769
P	1.717338	-0.007073	-0.570150
P	-1.403059	0.369855	-0.878782
C	-0.414931	0.409256	-2.465635
C	1.044099	-0.072206	-2.303689
H	-0.926381	-0.228700	-3.198830
H	-0.460388	1.436837	-2.854762
H	1.121931	-1.140442	-2.558053
H	1.719289	0.464717	-2.987147
C	3.415974	-0.703899	-0.749211
C	4.538486	0.128158	-0.892484
C	3.610522	-2.106462	-0.760401
C	5.823601	-0.401969	-1.026781
H	4.411052	1.211366	-0.897833
C	4.901909	-2.640096	-0.887063
C	5.999626	-1.786221	-1.017782
H	6.679724	0.266916	-1.136383
H	5.056766	-3.718491	-0.887452
H	7.000226	-2.214453	-1.116434
C	2.066234	1.759804	-0.210460
C	1.816915	2.799729	-1.117579
C	2.601127	2.072074	1.052831
C	2.092595	4.126035	-0.768210
H	1.408158	2.590720	-2.106517
C	2.889180	3.393581	1.394703
H	2.809009	1.272350	1.768281
C	2.630355	4.425908	0.485019
H	1.885721	4.925976	-1.482781
H	3.318161	3.620314	2.374072
H	2.849128	5.462038	0.754223
C	-1.370392	2.096103	-0.257581
C	-1.865727	3.152391	-1.037455
C	-0.870153	2.371855	1.030757
C	-1.858538	4.463711	-0.565486
H	-2.273476	2.935939	-2.028564
C	-0.869172	3.687832	1.513263
C	-1.357751	4.722135	0.712823
H	-2.245964	5.275155	-1.184907
H	-0.478676	3.922196	2.501252
H	-1.344377	5.743314	1.100999
C	-3.166946	0.139573	-1.322853
C	-4.129044	0.543504	-0.376430
C	-3.593538	-0.512936	-2.490447
C	-5.485181	0.300127	-0.597750
H	-3.819956	1.057854	0.536814
C	-4.953754	-0.752838	-2.708373
H	-2.876309	-0.848994	-3.241055
C	-5.901625	-0.350159	-1.764289
H	-6.220074	0.621671	0.144167
H	-5.271001	-1.259320	-3.623116
H	-6.963489	-0.540800	-1.937374
O	2.494995	-2.865871	-0.655223
O	-0.388126	1.314052	1.775786
C	2.594065	-4.281764	-0.642589
H	1.567547	-4.659549	-0.558016
H	3.042564	-4.664318	-1.575300
H	3.183428	-4.637250	0.220102
C	-0.030226	1.567523	3.139213
H	0.801897	2.283631	3.199330
H	-0.896515	1.947447	3.702691
H	0.289018	0.614485	3.570823
C	-1.818539	-1.333697	2.355248
C	-2.662349	-2.532352	2.762638
C	-2.766045	-3.669969	1.732815
C	-3.081516	-3.196113	0.299090
C	-1.880891	-3.188547	-0.665894
C	-0.529805	-2.676788	-0.153181
H	-1.847035	-0.548094	3.122409
H	-2.269084	-0.893136	1.444363
H	-2.313413	-2.937717	3.729140
H	-3.685108	-2.156636	2.960352
H	-1.836127	-4.264116	1.730193
H	-3.549231	-4.361682	2.083088
H	-3.532627	-2.190090	0.336189
H	-3.861193	-3.837687	-0.142750
H	-1.726533	-4.229583	-1.015647
H	-2.175654	-2.630399	-1.569987
H	-0.087535	-3.410432	0.542157
H	0.168198	-2.617898	-1.002285
C	1.300617	-1.628934	2.270149
C	0.154419	-2.093676	2.937980
H	1.870784	-0.794605	2.692781
H	1.863601	-2.306892	1.624647
H	-0.148637	-3.131973	2.792993
H	-0.104948	-1.690357	3.919713

^{4}TS9-10B-23
Geometry with 85 atoms:
Total energy: -3274.475694510

Cr	-0.537285	-0.772627	0.897495
P	1.606673	-0.339171	-0.403669
P	-1.404285	0.565254	-1.055614
C	-0.152918	0.728552	-2.437928
C	1.125911	-0.088437	-2.191223
H	-0.622910	0.429567	-3.386243
H	0.066854	1.800939	-2.533741
H	0.985854	-1.122702	-2.546040
H	1.981599	0.329316	-2.739514
C	2.977511	-1.548078	-0.509234
C	2.863949	-2.804891	0.101524
C	4.174429	-1.228499	-1.202950
C	3.905038	-3.735319	0.047057
H	1.944905	-3.057488	0.628840
C	5.223593	-2.158604	-1.248175
C	5.081516	-3.402555	-0.625802
H	3.795684	-4.708901	0.528924
H	6.149207	-1.922859	-1.773131
H	5.906596	-4.117827	-0.673924
C	2.405511	1.199933	0.203428
C	3.320501	1.105823	1.267066
C	2.055198	2.469749	-0.280213
C	3.883379	2.257745	1.821524
H	3.612152	0.126749	1.655391
C	2.616866	3.621448	0.279130
H	1.333493	2.577519	-1.089465
C	3.533703	3.520199	1.329957
H	4.602004	2.167987	2.640187
H	2.333362	4.602089	-0.110945
H	3.975962	4.420673	1.763000
C	-1.650549	2.268180	-0.445815
C	-2.318116	3.243650	-1.204125
C	-1.110408	2.620397	0.810038
C	-2.457107	4.549237	-0.733826
H	-2.741651	2.966892	-2.173065
C	-1.250148	3.932787	1.284610
C	-1.920528	4.884155	0.511912

H -2.979883 5.297697 -1.332734
H -0.840238 4.226688 2.249099
H -2.022135 5.901769 0.896749
C -2.992229 0.037936 -1.783770
C -4.202093 0.429265 -1.180385
C -3.018251 -0.919905 -2.813753
C -5.413298 -0.113850 -1.615982
H -4.201906 1.162567 -0.371085
C -4.233501 -1.457367 -3.245570
H -2.092774 -1.264151 -3.281884
C -5.432607 -1.056927 -2.648330
H -6.346745 0.202422 -1.144023
H -4.241120 -2.196618 -4.050207
H -6.381203 -1.480923 -2.986146
O 4.222306 -0.013109 -1.790949
O -0.449757 1.643429 1.521153
C 5.428261 0.453813 -2.374202
H 5.227908 1.479488 -2.711461
H 6.251205 0.471999 -1.639162
H 5.725950 -0.158520 -3.242909
C 0.219919 2.037030 2.724864
H 0.940184 2.842162 2.521149
H -0.506338 2.353766 3.489982
H 0.769542 1.164888 3.086571
C -2.438841 -0.755447 1.981323
C -3.428954 -1.625606 2.740910
C -3.355958 -3.146851 2.506200
C -3.038529 -3.633236 1.080645
C -1.541658 -3.744342 0.702813
C -0.912802 -2.571694 -0.056383
H -2.526961 0.300618 2.278554
H -2.701113 -0.829120 0.909051
H -3.358860 -1.427385 3.825377
H -4.439377 -1.278124 2.452114
H -2.620507 -3.604315 3.191610
H -4.326233 -3.567115 2.818723
H -3.568816 -3.012822 0.334883
H -3.476524 -4.639937 0.983083
H -0.954353 -3.981912 1.609610
H -1.433273 -4.639941 0.061358
H 0.060939 -2.888649 -0.468578
H -1.552395 -2.331888 -0.924687
C 0.623567 -1.447575 2.583478
C -0.638649 -1.352574 3.186702
H 1.385741 -0.681038 2.756128
H 1.012728 -2.439278 2.341251
H -1.160140 -2.272413 3.441986
H -0.878029 -0.501473 3.829968

^{4}TS9-10B-24
Geometry with 85 atoms:
Total energy: -3274.478466110
Cr -0.066427 -0.901170 1.015010
P 1.323556 0.698080 -0.634132
P -1.678592 -0.343586 -0.765885
C -0.863868 0.132799 -2.387411
C 0.670670 0.212914 -2.308596
H -1.162836 -0.594754 -3.155068
H -1.300509 1.096192 -2.684146
H 1.119026 -0.774875 -2.485340
H 1.071537 0.887474 -3.080667
C 3.151178 0.819198 -0.869150
C 3.851489 2.016969 -0.658069
C 3.887177 -0.333815 -1.238401
C 5.240646 2.081718 -0.798460
H 3.306918 2.920916 -0.382947
C 5.279294 -0.268941 -1.387020
C 5.949260 0.937086 -1.162424
H 5.760662 3.026921 -0.629147
H 5.847487 -1.153045 -1.674629
H 7.035202 0.974210 -1.278528
C 0.816487 2.447278 -0.388539
C 0.273326 3.250364 -1.403587
C 0.970898 2.993922 0.898394
C -0.126287 4.562774 -1.131215
H 0.159232 2.866127 -2.418234
C 0.590252 4.309609 1.164881
H 1.399961 2.386375 1.699428
C 0.029724 5.094716 0.150903
H -0.557666 5.172217 -1.928859
H 0.728917 4.724338 2.166553
H -0.280431 6.121344 0.359948
C -2.567582 1.169213 -0.250728
C -3.538621 1.749510 -1.083415
C -2.270208 1.778829 0.986112
C -4.208339 2.913180 -0.710111
H -3.778820 1.268701 -2.035463
C -2.950526 2.945489 1.367822
C -3.907702 3.504482 0.519484
H -4.961265 3.351097 -1.368513
H -2.736432 3.433904 2.316144
H -4.423911 4.415863 0.830660
C -2.985734 -1.553658 -1.181917
C -2.739412 -2.576898 -2.114111
C -4.197085 -1.554263 -0.467624
C -3.694776 -3.571874 -2.338245
H -1.800221 -2.608212 -2.671353
C -5.147950 -2.551583 -0.695438
H -4.403419 -0.769741 0.263554
C -4.900525 -3.561324 -1.630990
H -3.493631 -4.358891 -3.069110
H -6.088386 -2.537730 -0.139099
H -5.646616 -4.339728 -1.807992
O 3.166917 -1.467753 -1.434704
O -1.307292 1.195727 1.775908
C 3.807869 -2.644532 -1.902084
H 4.285868 -2.477347 -2.882712
H 4.562536 -3.009698 -1.185881
H 3.021207 -3.402361 -2.009435
C -1.157911 1.679995 3.112685
H -0.371186 1.082852 3.583418
H -0.846429 2.734861 3.122281
H -2.096302 1.559798 3.677662
C 1.267781 -0.888221 2.776558
C 2.533322 -1.554294 2.224874
C 2.664481 -3.061696 2.507301
C 2.258768 -3.989783 1.355676
C 0.812209 -3.926754 0.846588
C 0.405051 -2.677411 0.054292
H 1.265952 0.199223 2.564010
H 1.281599 -0.964257 3.868666
H 2.650102 -1.377545 1.144185
H 3.382061 -1.022682 2.695967
H 3.718265 -3.281452 2.746931
H 2.099818 -3.322918 3.420245
H 2.465082 -5.026796 1.673539
H 2.934929 -3.799466 0.503819
H 0.675654 -4.802699 0.182541
H 0.114586 -4.110873 1.683591
H 1.192405 -2.411081 -0.668022
H -0.507876 -2.914647 -0.516721
C -1.625699 -1.835223 2.096430
C -0.635908 -1.848892 3.109726
H -1.860948 -2.762037 1.566625
H -2.457428 -1.132239 2.202756
H -0.781217 -1.199160 3.975832
H -0.131173 -2.786605 3.348737

^{4}TS9-10B-25
Geometry with 85 atoms:
Total energy: -3274.475014830
Cr -0.499493 -0.826707 1.149478
P 1.536024 -0.296687 -0.384777
P -1.590023 0.348685 -0.819431
C -0.517794 0.015148 -2.301180
C 0.939833 0.387305 -2.022529
H -0.610899 -1.061597 -2.516667
H -0.902384 0.564484 -3.174793
H 1.600311 0.015968 -2.816826
H 1.057239 1.478889 -2.002995
C 2.720560 -1.625671 -0.829764
C 2.561464 -2.939434 -0.366645
C 3.857004 -1.315233 -1.624037
C 3.497293 -3.933481 -0.666365
H 1.691314 -3.195575 0.235884
C 4.800977 -2.310189 -1.916050
C 4.614908 -3.610172 -1.436626
H 3.352696 -4.949967 -0.295128
H 5.678542 -2.079658 -2.519915
H 5.357412 -4.376022 -1.674517
C 2.615626 1.001095 0.356780
C 2.411022 2.371807 0.137975
C 3.627987 0.602661 1.249411
C 3.196222 3.322286 0.798497
H 1.640586 2.721951 -0.549076
C 4.410790 1.553718 1.907553
H 3.819172 -0.458625 1.423495
C 4.195975 2.918606 1.687365
H 3.022108 4.384896 0.610974
H 5.196834 1.225039 2.591995
H 4.810713 3.662510 2.199974
C -1.317886 2.127165 -0.466613
C -1.644112 3.110673 -1.415079
C -0.778353 2.523547 0.774058
C -1.440162 4.464146 -1.152084
H -2.075962 2.803488 -2.371149
C -0.581220 3.886004 1.046766
C -0.910894 4.842716 0.084841
H -1.697250 5.216292 -1.900529
H -0.157294 4.215012 1.993167
H -0.747944 5.899129 0.311620
C -3.307069 0.288051 -1.448451
C -3.657928 -0.522548 -2.540781
C -4.314641 0.987647 -0.759070
C -4.995049 -0.630591 -2.934499
H -2.898675 -1.081463 -3.090762
C -5.647509 0.875811 -1.157017
H -4.059158 1.624228 0.091939
C -5.991523 0.063754 -2.243383
H -5.256890 -1.262736 -3.786483
H -6.422150 1.424428 -0.615697
H -7.035836 -0.024930 -2.552207
O 3.951255 -0.039429 -2.058017
O -0.441157 1.534888 1.677361
C 5.135683 0.418525 -2.690640
H 4.994636 1.494136 -2.861394
H 6.018699 0.269319 -2.045976
H 5.300708 -0.081369 -3.660652
C 0.090327 1.950362 2.943236
H -0.624691 2.600904 3.469647
H 0.244687 1.047369 3.537029
H 1.053771 2.464277 2.808573
C -2.100557 -1.108728 2.683435
C -2.784654 -2.459536 2.929858
C -3.916529 -2.827759 1.954691
C -3.639022 -2.526083 0.478985
C -2.357879 -3.086496 -0.162434
C -0.972972 -2.702292 0.398606
H -2.211476 -0.402730 3.515854
H -2.543392 -0.590798 1.809985
H -2.042091 -3.272641 2.885888
H -3.176826 -2.490833 3.960208
H -4.142999 -3.900663 2.085005
H -4.837650 -2.286985 2.236080
H -3.656292 -1.437065 0.340724
H -4.496989 -2.890901 -0.111609
H -2.431816 -4.191920 -0.180990
H -2.391753 -2.782706 -1.223855
H -0.693472 -3.352232 1.246825
H -0.228361 -2.891020 -0.392647
C 1.042636 -1.357491 2.581427
C -0.066741 -1.555607 3.415170
H 1.680368 -0.482621 2.734955
H 1.541036 -2.228332 2.149754
H -0.408718 -2.573017 3.609265
H -0.247715 -0.866885 4.243488

^{4}TS9-10C-01
Geometry with 89 atoms:
Total energy: -3202.740275190
Cr 0.268563 0.094226 1.387755
P -1.578396 0.274491 -0.598485
P 1.762741 0.470263 -0.616308
C 0.730623 0.315827 -2.154538
C -0.594497 1.064421 -1.971631
H 1.286876 0.676082 -3.032481
H 0.553470 -0.756000 -2.324780
H -0.404598 2.114186 -1.702770
H -1.183006 1.062810 -2.901792
C -3.011056 1.402078 -0.325823
C -3.053540 2.673333 -0.930182
C -4.047116 1.021519 0.564636
C -4.096844 3.562748 -0.667379

H -2.269961 2.989354 -1.619170
C -5.084884 1.933881 0.812327
C -5.117490 3.191914 0.210112
H -4.107866 4.543562 -1.148483
H -5.884274 1.645200 1.500766
H -5.936672 3.881528 0.427716
C -2.297807 -1.186218 -1.459784
C -1.965938 -2.486411 -1.052810
C -3.194002 -1.010819 -2.529633
C -2.520208 -3.595490 -1.701142
H -1.272389 -2.643188 -0.225623
C -3.742447 -2.117739 -3.178993
H -3.480267 -0.003591 -2.843698
C -3.407665 -3.412684 -2.764246
H -2.257845 -4.604096 -1.372636
H -4.440533 -1.970766 -4.006743
H -3.842900 -4.278160 -3.269650
C 3.238114 -0.609784 -0.861371
C 3.121060 -2.021383 -0.832771
C 4.510211 -0.022409 -1.002067
C 4.292627 -2.789087 -0.936087
C 5.657488 -0.807749 -1.110703
C 5.548935 -2.199532 -1.071361
H 4.210428 -3.879285 -0.907627
H 6.633576 -0.329675 -1.221368
H 6.441343 -2.825854 -1.145009
C 2.409842 2.195304 -0.672842
C 2.991835 2.742266 0.486648
C 2.351752 2.986776 -1.833044
C 3.504352 4.040693 0.482718
H 3.054417 2.151210 1.400899
C 2.855797 4.291422 -1.830744
H 1.920261 2.600177 -2.757066
C 3.433969 4.821690 -0.675147
H 3.958251 4.443931 1.391153
H 2.799801 4.891652 -2.742178
H 3.829833 5.840110 -0.676221
C -0.996276 -0.490183 3.141487
C -0.672862 -1.820355 2.455263
C 0.084692 -2.836599 3.326255
C 1.401108 -2.334898 3.935589
C 2.351097 -1.617420 2.965585
C 1.955956 -0.181726 2.588427
H -0.448902 -0.396986 4.082778
H -2.070154 -0.424342 3.331603
H -1.596888 -2.268001 2.060407
H -0.042656 -1.758644 1.512576
H -0.589897 -3.172870 4.131419
H 0.285954 -3.725490 2.702838
H 1.913996 -3.208097 4.371662
H 1.192422 -1.664300 4.787655
H 3.351407 -1.596289 3.437653
H 2.484835 -2.231858 2.055305
H 1.783579 0.417578 3.502365
H 2.809306 0.283854 2.070332
C -0.068292 2.096109 1.830289
C -1.017262 1.551669 2.744350
H -0.452074 2.593364 0.932145
H 0.849239 2.531025 2.235260
H -0.851199 1.697238 3.814094
H -2.069866 1.595773 2.453276
H 4.611287 1.063149 -1.023986
C 1.798467 -2.755413 -0.744802
C 1.396222 -3.434064 -2.060971
H 1.000207 -2.066653 -0.426723
H 1.866319 -3.520034 0.047247
H 0.429520 -3.950642 -1.962545
H 1.307724 -2.705527 -2.882393
H 2.149531 -4.176947 -2.365255
C -4.105888 -0.333245 1.241307
C -5.145198 -1.282015 0.629258
H -4.342316 -0.183074 2.308495
H -3.117276 -0.813014 1.214116
H -4.929859 -1.483129 -0.430188
H -5.155055 -2.245152 1.164214
H -6.157081 -0.851401 0.691092

[4]TS9-10C-02
Geometry with 89 atoms:
Total energy: -3202.741367870
Cr 0.135632 -1.330740 0.675795
P 1.561345 0.387679 -0.764743
P -1.674813 -0.057010 -0.505339
C -0.935096 1.006563 -1.858353
C 0.474863 0.567695 -2.268636
H -1.603744 1.019955 -2.730931
H -0.910263 2.029392 -1.454666
H 0.446446 -0.402007 -2.786553
H 0.919803 1.301186 -2.959354
C 3.219182 -0.071493 -1.414569
C 3.337176 -0.578365 -2.723121
C 4.368250 -0.006188 -0.581097
C 4.565180 -1.018829 -3.218575
H 2.467210 -0.633950 -3.378541
C 5.591581 -0.450172 -1.107671
C 5.697426 -0.952290 -2.406038
H 4.633206 -1.406735 -4.237649
H 6.488792 -0.400958 -0.487935
H 6.666660 -1.289269 -2.781633
C 1.681004 2.140355 -0.218083
C 2.530750 3.058221 -0.858479
C 0.867416 2.579858 0.838505
C 2.565414 4.390935 -0.440902
H 3.174810 2.729920 -1.678457
C 0.897069 3.915842 1.248699
H 0.194109 1.883660 1.342175
C 1.749556 4.821911 0.612042
H 3.233402 5.097645 -0.939532
H 0.253133 4.244795 2.067998
H 1.780326 5.865084 0.935893
C -2.697899 1.065150 0.532616
C -3.732314 1.902742 0.045885
C -2.403864 1.054666 1.909888
C -4.423619 2.698880 0.976265
C -3.099185 1.857916 2.811975
C -4.118466 2.686750 2.337322
H -5.229337 3.343959 0.614743
H -2.853978 1.826580 3.876112
H -4.682464 3.318700 3.027881
C -2.843338 -1.189010 -1.349931
C -4.042251 -1.571844 -0.724701
C -2.506562 -1.753483 -2.592538
C -4.891794 -2.495706 -1.339038
H -4.323182 -1.138811 0.237818
C -3.361042 -2.674494 -3.203604
H -1.575411 -1.481111 -3.093681
C -4.554812 -3.048204 -2.578301
H -5.824433 -2.781066 -0.846293
H -3.091758 -3.102146 -4.172490
H -5.222280 -3.768333 -3.057588
C 1.957738 -2.119555 1.639881
C 1.454319 -1.073016 2.641724
C 1.058534 -1.611549 4.021235
C -0.027499 -2.691316 4.028103
C -1.327117 -2.281473 3.323205
C -1.293728 -2.383154 1.793992
H 2.201742 -3.042671 2.174309
H 2.843481 -1.766250 1.105504
H 2.233806 -0.302738 2.751696
H 0.592486 -0.416940 2.286153
H 1.972597 -2.000786 4.501328
H 0.724829 -0.760052 4.639619
H -0.237482 -2.945490 5.080174
H 0.356919 -3.619734 3.568430
H -2.142318 -2.926379 3.702517
H -1.602751 -1.259569 3.645996
H -1.142183 -3.441492 1.513169
H -2.284945 -2.113937 1.391758
C 0.291044 -2.793063 -0.799075
C 1.241130 -3.336716 0.114767
H 0.670079 -2.403109 -1.749496
H -0.701070 -3.251281 -0.853407
H 0.908716 -4.151528 0.762281
H 2.280342 -3.428304 -0.211346
H -1.626741 0.388115 2.284989
C -4.128529 2.017672 -1.412296
C -3.681341 3.338644 -2.054729
H -5.226956 1.943223 -1.478107
H -3.743697 1.168540 -1.991425
H -4.123238 4.204109 -1.536076
H -2.587343 3.458335 -2.018076
H -3.993657 3.383980 -3.110173
C 4.310994 0.562226 0.825643
C 5.207799 -0.116546 1.862713
H 3.272306 0.534329 1.184812
H 4.553004 1.639029 0.777187
H 6.277777 0.026436 1.649045
H 5.022697 0.309144 2.861556
H 5.019586 -1.201123 1.914073

[4]TS9-10C-03
Geometry with 89 atoms:
Total energy: -3202.742044400
Cr 0.045424 -1.419703 0.699737
P 1.594178 0.205008 -0.714191
P -1.650272 -0.038787 -0.529792
C -0.820097 0.938532 -1.894058
C 0.566791 0.397741 -2.257424
H -1.469494 0.968960 -2.780514
H -0.737233 1.967128 -1.514118
H 0.491430 -0.583848 -2.747656
H 1.071458 1.082074 -2.957487
C 3.259746 -0.313737 -1.296530
C 3.418083 -0.821757 -2.601564
C 4.369658 -0.303978 -0.413900
C 4.647989 -1.313302 -3.040404
H 2.578968 -0.837376 -3.298259
C 5.596217 -0.803545 -0.881255
C 5.743388 -1.305530 -2.174175
H 4.747209 -1.699046 -4.057763
H 6.455823 -0.800254 -0.205095
H 6.711097 -1.690955 -2.504260
C 1.744775 1.965588 -0.205024
C 2.486112 2.883155 -0.969006
C 1.042466 2.419303 0.921849
C 2.521465 4.231495 -0.606627
H 3.045204 2.543088 -1.844718
C 1.076572 3.769933 1.281719
H 0.453486 1.722854 1.521741
C 1.817041 4.676666 0.518561
H 3.102938 4.938511 -1.203433
H 0.519402 4.110875 2.157680
H 1.846526 5.732349 0.799157
C -2.568319 1.182679 0.491554
C -3.507108 2.119065 -0.007920
C -2.275078 1.158516 1.868677
C -4.104289 3.000602 0.910628
C -2.876929 2.045492 2.759083
C -3.798545 2.975417 2.271415
H -4.835045 3.725048 0.540640
H -2.634894 2.003814 3.823589
H -4.287085 3.676849 2.952307
C -2.902382 -1.082818 -1.366307
C -4.155869 -1.317573 -0.777424
C -2.575560 -1.731799 -2.569713
C -5.070499 -2.177380 -1.391824
H -4.426817 -0.819344 0.156014
C -3.494415 -2.588234 -3.180889
H -1.600832 -1.575413 -3.037103
C -4.743680 -2.812935 -2.593365
H -6.045515 -2.347477 -0.928673
H -3.232149 -3.083466 -4.119051
H -5.461605 -3.483118 -3.072169
C 1.787028 -2.293161 1.736129
C 1.294518 -1.218740 2.711600
C 0.825081 -1.728614 4.079438
C -0.314958 -2.750456 4.050085
C -1.565974 -2.275528 3.298832
C -1.483808 -2.380860 1.771552
H 1.963064 -3.224867 2.282057
H 2.709513 -1.985825 1.235681
H 2.098155 -0.477429 2.842555
H 0.466251 -0.538489 2.324628
H 1.700394 -2.161193 4.593379
H 0.513707 -0.857525 4.682185
H -0.574997 -2.989600 5.094505
H 0.036519 -3.699207 3.605589
H -2.425981 -2.877617 3.648393
H -1.800307 -1.240784 3.613034
H -1.381121 -3.446981 1.497639
H -2.444032 -2.059948 1.334129
C 0.171913 -2.904408 -0.758416
C 1.060710 -3.486705 0.191981

H	0.602895	-2.547804	-1.699798
H	-0.841437	-3.309284	-0.840654
H	0.665329	-4.275707	0.835889
H	2.104482	-3.634218	-0.096819
H	-1.568794	0.418400	2.247663
C	-3.896820	2.247430	-1.467143
C	-3.337668	3.511393	-2.136079
H	-4.997983	2.271125	-1.527547
H	-3.592663	1.357672	-2.033510
H	-3.657478	3.567386	-3.188797
H	-3.691716	4.422917	-1.629198
H	-2.236987	3.530460	-2.114465
C	4.311392	0.240091	1.000864
C	5.081061	1.554096	1.186585
H	4.725746	-0.519429	1.686013
H	3.268280	0.394070	1.311451
H	6.145742	1.431596	0.933007
H	4.670667	2.348964	0.546679
H	5.021088	1.894827	2.232500

^{4}TS9-10C-04
Geometry with 89 atoms:
Total energy: -3202.739450420

Cr	0.253987	1.379267	-0.914516
P	-1.638796	-0.379958	-0.091450
P	1.640017	-0.589411	-0.267487
C	0.557346	-2.086905	-0.462592
C	-0.712464	-1.939990	0.380612
H	0.300613	-2.149596	-1.532248
H	1.099942	-3.007568	-0.210167
H	-1.363956	-2.812011	0.238514
H	-0.470802	-1.890630	1.453461
C	-3.058252	-0.924943	-1.125787
C	-3.128098	-0.352863	-2.411129
C	-4.064135	-1.834876	-0.708093
C	-4.163537	-0.662730	-3.292246
H	-2.358816	0.352916	-2.721053
C	-5.101960	-2.122037	-1.611678
C	-5.158987	-1.552921	-2.884343
H	-4.194562	-0.208001	-4.285043
H	-5.891177	-2.811646	-1.300274
H	-5.984940	-1.802285	-3.555116
C	-2.367503	0.283867	1.459865
C	-3.653855	0.851442	1.460900
C	-1.574460	0.389616	2.616660
C	-4.137451	1.501597	2.600206
H	-4.285097	0.782189	0.571923
C	-2.063312	1.038323	3.753229
H	-0.563069	-0.021457	2.639707
C	-3.345170	1.598171	3.748466
H	-5.141572	1.932805	2.589517
H	-1.435571	1.107060	4.645298
H	-3.725856	2.106812	4.637379
C	2.238324	-0.579502	1.473630
C	2.934721	-1.638462	2.109918
C	1.981269	0.607607	2.188423
C	3.325199	-1.456661	3.448289
C	2.377110	0.763387	3.515902
C	3.053109	-0.281716	4.149638
H	3.867208	-2.264401	3.948215
H	2.165989	1.695642	4.044739
H	3.378643	-0.179627	5.187859
C	3.103725	-0.873593	-1.328177
C	4.371025	-0.424939	-0.916659
C	2.960922	-1.452533	-2.601974
C	5.475345	-0.564622	-1.760803
H	4.500741	0.026500	0.069446
C	4.070298	-1.593391	-3.439659
H	1.986024	-1.796511	-2.953542
C	5.329027	-1.150345	-3.021867
H	6.455911	-0.215336	-1.428338
H	3.948547	-2.051063	-4.424502
H	6.194671	-1.260790	-3.679346
C	-1.290798	2.899527	-1.349353
C	-0.995270	3.126328	0.136752
C	-0.409034	4.493741	0.499773
C	0.915367	4.850184	-0.180984
C	2.030655	3.816929	0.031506
C	1.966501	2.593982	-0.890313
H	-1.306989	3.861311	-1.871159
H	-2.252702	2.393080	-1.487900
H	-1.923152	2.946942	0.701628
H	-0.332312	2.345506	0.631635
H	-1.167934	5.258602	0.261942
H	-0.272632	4.526015	1.594814
H	1.237152	5.830740	0.207138
H	0.758515	4.996001	-1.265136
H	3.002597	4.322718	-0.123555
H	2.038400	3.510853	1.095252
H	2.095747	2.928765	-1.935812
H	2.829831	1.938663	-0.686140
C	0.393817	0.936051	-2.946070
C	-0.332669	2.156037	-3.057178
H	-0.127792	0.002457	-3.185664
H	1.463748	0.945089	-3.174498
H	0.234295	3.061039	-3.287360
H	-1.325757	2.144159	-3.513670
H	1.467756	1.431131	1.689221
C	3.272334	-2.962415	1.453978
C	2.416720	-4.125745	1.976365
H	4.333999	-3.184945	1.652906
H	3.189383	-2.892539	0.361575
H	2.680971	-5.065094	1.465266
H	2.566099	-4.277530	3.056933
H	1.340989	-3.944459	1.820056
C	-4.097140	-2.520491	0.645157
C	-3.951399	-4.046389	0.560598
H	-5.059075	-2.279800	1.129624
H	-3.327932	-2.112328	1.312484
H	-3.008410	-4.339026	0.070117
H	-3.964259	-4.493422	1.567260
H	-4.771337	-4.501136	-0.016717

^{4}TS9-10C-05
Geometry with 89 atoms:
Total energy: -3202.739214900

Cr	-0.013793	-0.760969	1.249088
P	-1.719772	-0.193813	-0.468107
P	1.588598	0.131228	-0.715823
C	0.407833	0.511261	-2.114429
C	-0.857277	-0.351054	-2.111050
H	0.140567	1.569487	-1.965349
H	0.931471	0.457869	-3.081297
H	-1.528243	-0.055983	-2.930831
H	-0.615072	-1.414759	-2.252424
C	-2.355577	1.531354	-0.428778
C	-1.812663	2.346840	0.584408
C	-3.262703	2.089625	-1.365462
C	-2.127757	3.700945	0.680765
H	-1.131031	1.905729	1.315659
C	-3.553374	3.461070	-1.254900
C	-2.999112	4.261554	-0.255891
H	-1.694962	4.311195	1.476667
H	-4.236698	3.911737	-1.979817
H	-3.251076	5.323866	-0.207877
C	-3.161999	-1.316806	-0.515942
C	-3.115524	-2.541963	-1.203314
C	-4.302321	-0.999601	0.243671
C	-4.200128	-3.421754	-1.146673
H	-2.239880	-2.823689	-1.790675
C	-5.381289	-1.884790	0.299863
H	-4.352680	-0.053043	0.786962
C	-5.334163	-3.096233	-0.396726
H	-4.156439	-4.367638	-1.692107
H	-6.263846	-1.623627	0.888859
H	-6.179752	-3.786946	-0.354326
C	2.734293	-1.161770	-1.360410
C	3.898429	-1.522646	-0.635726
C	2.395470	-1.880993	-2.522904
C	4.677488	-2.588536	-1.115209
C	3.184386	-2.938805	-2.976735
C	4.332873	-3.295413	-2.267086
H	5.576296	-2.872129	-0.560522
H	2.900770	-3.480199	-3.882325
H	4.958362	-4.123891	-2.608112
C	2.551885	1.695866	-0.686691
C	2.223799	2.682837	0.256923
C	3.546401	1.961355	-1.642984
C	2.885418	3.914137	0.251116
H	1.440942	2.496150	0.994813
C	4.205981	3.193108	-1.646292
H	3.812860	1.201889	-2.382082
C	3.879443	4.168975	-0.698364
H	2.623736	4.675421	0.990011
H	4.980369	3.390631	-2.391626
H	4.399883	5.129776	-0.701486
C	1.509144	-1.254439	2.801450
C	1.291960	0.258806	2.938954
C	0.798201	0.719805	4.320792
C	-0.492302	0.052301	4.819745
C	-1.644870	-0.010070	3.805315
C	-1.488670	-1.057251	2.692886
H	1.088083	-1.778132	3.662576
H	2.578009	-1.465148	2.732666
H	2.211565	0.793841	2.658596
H	0.545371	0.733471	2.224917
H	1.606850	0.551654	5.051608
H	0.649420	1.813084	4.273363
H	-0.820732	0.602820	5.716708
H	-0.276346	-0.972944	5.168871
H	-2.569890	-0.228686	4.371924
H	-1.810638	0.997073	3.375090
H	-1.266083	-2.044909	3.138553
H	-2.446306	-1.177219	2.163144
C	0.069326	-2.711299	0.552968
C	1.157489	-2.791357	1.478172
H	0.327917	-2.711895	-0.512428
H	-0.868080	-3.218443	0.804706
H	1.053990	-3.454024	2.340345
H	2.161815	-2.784084	1.049249
H	1.505928	-1.618103	-3.096494
C	4.359844	-0.815990	0.625493
C	5.651166	-0.007369	0.446864
H	4.524536	-1.576895	1.407793
H	3.570612	-0.153210	1.008439
H	6.481978	-0.649683	0.114801
H	5.522840	0.790330	-0.298972
H	5.948887	0.462383	1.397858
C	-3.956995	1.305952	-2.464388
C	-5.482970	1.253309	-2.305419
H	-3.581218	0.277040	-2.512292
H	-3.710874	1.773814	-3.433752
H	-5.764564	0.763407	-1.361278
H	-5.931770	2.258706	-2.311043
H	-5.935039	0.680183	-3.130280

^{4}TS9-10C-06
Geometry with 89 atoms:
Total energy: -3202.741941120

Cr	-0.327271	-0.932323	1.002688
P	1.542004	0.127637	-0.692441
P	-1.808302	0.038778	-0.791222
C	-0.792066	-0.082968	-2.343562
C	0.521883	0.683681	-2.164036
H	-0.603505	-1.147808	-2.542562
H	-1.366415	0.321565	-3.191865
H	1.130529	0.649634	-3.080569
H	0.312629	1.748295	-1.972549
C	2.706377	-1.145379	-1.352128
C	2.419863	-1.786115	-2.573041
C	3.829993	-1.565069	-0.595447
C	3.222611	-2.820288	-3.056266
H	1.559227	-1.480911	-3.169566
C	4.623999	-2.605675	-1.105789
C	4.332820	-3.233024	-2.316962
H	2.979233	-3.299523	-4.007485
H	5.494205	-2.931020	-0.528416
H	4.969529	-4.043010	-2.680854
C	2.573285	1.628674	-0.430061
C	2.571762	2.283964	0.809988
C	3.355373	2.143780	-1.478295
C	3.339097	3.437218	1.001908
H	1.975659	1.891070	1.635052
C	4.116234	3.299015	-1.287339
H	3.384889	1.632339	-2.443757
C	4.109904	3.946898	-0.046735
H	3.334791	3.937376	1.973429
H	4.722673	3.691028	-2.107476
H	4.710034	4.847691	0.102925
C	-2.432706	1.778754	-0.875933
C	-1.960841	2.824153	-0.050443
C	-3.393240	2.058988	-1.871486
C	-2.478871	4.117576	-0.253949

C	-3.891691	3.345800	-2.052693
C	-3.430081	4.383275	-1.235348
H	-2.116132	4.932675	0.378551
H	-4.636811	3.538556	-2.828090
H	-3.810215	5.399376	-1.366693
C	-3.308717	-0.972654	-1.076235
C	-3.346046	-2.016103	-2.016115
C	-4.432292	-0.747936	-0.259086
C	-4.486912	-2.816914	-2.136163
H	-2.493246	-2.217276	-2.666545
C	-5.568102	-1.548858	-0.383556
H	-4.426529	0.064061	0.471771
C	-5.598113	-2.586848	-1.321487
H	-4.505063	-3.622051	-2.874832
H	-6.434886	-1.359959	0.254374
H	-6.488248	-3.213094	-1.418043
C	1.130569	-1.805353	2.399807
C	0.870932	-0.442812	3.068250
C	0.260067	-0.495142	4.477263
C	-1.261813	-0.674373	4.551481
C	-1.860384	-1.748699	3.632161
C	-2.005616	-1.319534	2.169218
H	1.074623	-2.590872	3.158488
H	2.118356	-1.830319	1.933807
H	1.838350	0.084868	3.096884
H	0.249600	0.286890	2.464730
H	0.760295	-1.311114	5.026483
H	0.530442	0.433637	5.007053
H	-1.750759	0.288429	4.321121
H	-1.520221	-0.896372	5.600071
H	-1.276901	-2.683878	3.716954
H	-2.863924	-2.002428	4.023595
H	-2.571706	-2.077645	1.602395
H	-2.610109	-0.393294	2.129186
C	-0.377709	-2.747436	-0.062883
C	0.252252	-3.224367	1.116634
H	0.230978	-2.692835	-0.972080
H	-1.434552	-2.983011	-0.214509
H	-0.375252	-3.711107	1.867749
H	1.260759	-3.637428	1.041298
H	-3.764625	1.253235	-2.508986
C	-0.952639	2.639948	1.062170
C	-1.582793	2.656817	2.459082
H	-0.192927	3.434924	0.990970
H	-0.405033	1.696948	0.917299
H	-2.095327	3.612445	2.650316
H	-2.326096	1.852886	2.570227
H	-0.817192	2.526245	3.240786
C	4.251422	-0.934681	0.718601
C	5.475747	-0.018156	0.594906
H	4.480727	-1.742894	1.433600
H	3.420653	-0.365711	1.160445
H	5.279157	0.821523	-0.086855
H	5.750520	0.397818	1.577186
H	6.345444	-0.571377	0.206824

^{4}TS9-10C-07
Geometry with 89 atoms:
Total energy: -3202.739491920

Cr	-0.084582	-1.115406	1.039840
P	1.530144	0.249832	-0.639681
P	-1.756406	-0.125010	-0.504117
C	-0.887017	0.041509	-2.137937
C	0.375026	0.889398	-1.966615
H	-0.640858	-0.979024	-2.467115
H	-1.553435	0.473674	-2.896394
H	0.917007	1.010007	-2.917027
H	0.106758	1.904333	-1.633860
C	2.731557	-0.846869	-1.510877
C	2.447098	-1.313687	-2.808804
C	3.886708	-1.322923	-0.840324
C	3.285144	-2.227018	-3.450209
H	1.560657	-0.968546	-3.342315
C	4.716446	-2.237975	-1.509203
C	4.428181	-2.691292	-2.796464
H	3.042967	-2.572262	-4.458091
H	5.609925	-2.606298	-0.997069
H	5.091984	-3.408182	-3.285682
C	2.449879	1.789572	-0.239995
C	2.134091	2.495038	0.932064
C	3.407430	2.315305	-1.123858
C	2.772387	3.704692	1.221691
H	1.383610	2.104433	1.622465
C	4.041571	3.525475	-0.833102
H	3.666633	1.772989	-2.036562
C	3.727687	4.219757	0.340721
H	2.522611	4.245246	2.137947
H	4.786656	3.926607	-1.524571
H	4.229187	5.163639	0.568069
C	-2.324965	1.562307	-0.033378
C	-3.186072	2.387814	-0.799568
C	-1.851595	2.023861	1.210449
C	-3.522077	3.649021	-0.276889
C	-2.193149	3.280893	1.705820
C	-3.036321	4.099305	0.951013
H	-4.190656	4.292697	-0.855641
H	-1.812451	3.612317	2.674595
H	-3.323918	5.086276	1.321790
C	-3.257952	-1.118270	-0.825318
C	-4.402941	-0.915855	-0.034249
C	-3.259877	-2.142425	-1.787923
C	-5.533577	-1.714962	-0.215853
H	-4.416351	-0.127712	0.722327
C	-4.395061	-2.938747	-1.964800
H	-2.382169	-2.326731	-2.410844
C	-5.533373	-2.726549	-1.181715
H	-6.419885	-1.544476	0.400102
H	-4.388683	-3.727734	-2.720887
H	-6.419992	-3.349072	-1.323701
C	1.413334	-1.923185	2.478929
C	1.103673	-0.504654	2.982362
C	0.547500	-0.432436	4.414832
C	-0.719437	-1.261316	4.673070
C	-1.835875	-1.116824	3.626724
C	-1.582766	-1.840654	2.295422
H	1.016412	-2.663159	3.177440
H	2.493841	-2.048919	2.387866
H	1.998357	0.127246	2.880582
H	0.342767	0.096152	2.386635
H	1.342435	-0.745269	5.112244
H	0.342063	0.629197	4.638848
H	-1.104292	-0.972675	5.665091
H	-0.458770	-2.330748	4.760328
H	-2.763421	-1.516585	4.078544
H	-2.046269	-0.042688	3.457043
H	-1.315317	-2.895677	2.493680
H	-2.514061	-1.872609	1.708378
C	0.083541	-2.835084	-0.096173
C	1.143817	-3.109192	0.826996
H	0.379036	-2.586861	-1.121576
H	-0.843898	-3.410512	-0.007441
H	1.030846	-3.960773	1.501504
H	2.160698	-2.987036	0.446778
H	-1.212538	1.370538	1.807460
C	-3.747929	2.016211	-2.156856
C	-3.081346	2.781691	-3.309483
H	-4.827361	2.242112	-2.157787
H	-3.677535	0.934453	-2.328983
H	-1.993869	2.606546	-3.342255
H	-3.505167	2.474451	-4.278770
H	-3.230748	3.868035	-3.206516
C	4.286413	-0.891832	0.558520
C	5.528829	0.007281	0.599473
H	4.486565	-1.798307	1.155228
H	3.452446	-0.377608	1.057912
H	6.398491	-0.496026	0.148485
H	5.360674	0.945845	0.052320
H	5.789016	0.261807	1.639293

^{4}TS9-10C-08
Geometry with 89 atoms:
Total energy: -3202.739933690

Cr	-0.001784	-1.039954	1.032418
P	1.505314	0.368135	-0.709591
P	-1.750112	-0.190124	-0.497921
C	-0.918508	-0.008324	-2.151474
C	0.290380	0.920633	-2.019639
H	-0.616384	-1.021588	-2.456447
H	-1.620843	0.360152	-2.910677
H	0.808398	1.061006	-2.980722
H	-0.034827	1.921578	-1.694816
C	2.742384	-0.679296	-1.587696
C	2.442535	-1.197934	-2.860742
C	3.947202	-1.065327	-0.939822
C	3.307968	-2.085915	-3.502588
H	1.522786	-0.915613	-3.374404
C	4.801956	-1.954550	-1.609469
C	4.493413	-2.464057	-2.872847
H	3.053028	-2.476901	-4.490349
H	5.734680	-2.261158	-1.133697
H	5.181861	-3.157396	-3.362033
C	2.341567	1.957733	-0.328861
C	1.857349	2.729476	0.740636
C	3.406733	2.445107	-1.103988
C	2.430673	3.970196	1.032476
H	1.021727	2.367079	1.343687
C	3.981803	3.683063	-0.805138
H	3.793025	1.853491	-1.937780
C	3.496335	4.446102	0.262535
H	2.045459	4.564865	1.864371
H	4.812656	4.054260	-1.410240
H	3.949770	5.413067	0.493727
C	-2.415128	1.467949	-0.051647
C	-3.313685	2.237958	-0.833085
C	-1.965798	1.976424	1.183965
C	-3.708932	3.492419	-0.335306
C	-2.368265	3.224827	1.654628
C	-3.247278	3.988652	0.883784
H	-4.405311	4.093085	-0.927211
H	-2.005392	3.591875	2.617447
H	-3.581110	4.968189	1.235000
C	-3.171307	-1.308409	-0.766317
C	-4.397513	-1.075606	-0.120980
C	-3.006943	-2.478223	-1.529341
C	-5.444984	-1.990965	-0.250128
H	-4.539452	-0.174814	0.480057
C	-4.059225	-3.388114	-1.657324
H	-2.057130	-2.691476	-2.024527
C	-5.279597	-3.147466	-1.018188
H	-6.395673	-1.797451	0.252784
H	-3.922534	-4.291113	-2.257284
H	-6.100424	-3.861779	-1.117586
C	1.557418	-1.661140	2.493816
C	1.162369	-0.235213	2.916090
C	0.593432	-0.117693	4.341156
C	-0.596531	-1.033694	4.664822
C	-1.736884	-1.044553	3.634990
C	-1.442719	-1.804558	2.333436
H	1.197333	-2.383581	3.229262
H	2.644562	-1.732451	2.421745
H	2.020760	0.440464	2.785144
H	0.386202	0.296101	2.276375
H	1.410771	-0.315189	5.054788
H	0.298832	0.935208	4.496877
H	-0.990992	-0.722039	5.646116
H	-0.244337	-2.070557	4.808108
H	-2.615677	-1.505697	4.124523
H	-2.049245	-0.004638	3.420693
H	-1.098847	-2.828374	2.573165
H	-2.374571	-1.926224	1.758439
C	0.283302	-2.794476	-0.015905
C	1.378931	-2.931161	0.900419
H	0.539504	-2.579679	-1.059861
H	-0.590544	-3.439605	0.122049
H	1.352898	-3.759849	1.611778
H	2.374950	-2.740385	0.493782
H	-1.296562	1.370115	1.796957
C	-3.856450	1.817189	-2.184073
C	-3.220556	2.591395	-3.348223
H	-4.944578	1.996006	-2.190516
H	-3.738830	0.736512	-2.337589
H	-3.419816	3.671397	-3.265565
H	-2.126192	2.464822	-3.371871
H	-3.624744	2.247322	-4.313463
C	4.325074	-0.518660	0.424899
C	5.210170	-1.414743	1.291937
H	3.403752	-0.281456	0.978231
H	4.821313	0.457920	0.286849
H	4.784384	-2.425169	1.404972
H	6.223241	-1.527311	0.876739
H	5.322772	-0.978557	2.296771

^{4}TS9-10C-09

Geometry with 89 atoms:
Total energy: -3202.739138150

Cr	0.469233	-1.122449	0.978066
P	-1.718744	-0.017094	-0.307623
P	1.512202	0.582511	-0.600545
C	0.418070	0.523444	-2.111049
C	-1.019083	0.932185	-1.760620
H	0.823421	1.194068	-2.885150
H	0.454935	-0.504526	-2.506696
H	-1.049853	1.992524	-1.473057
H	-1.671145	0.819182	-2.638460
C	-2.901127	1.091416	0.563878
C	-2.736682	1.161294	1.961174
C	-3.952569	1.815976	-0.051980
C	-3.569341	1.947685	2.756650
H	-1.943908	0.582859	2.433591
C	-4.778458	2.601385	0.771209
C	-4.595376	2.677336	2.152255
H	-3.419209	1.985152	3.838080
H	-5.594099	3.163944	0.308163
H	-5.260843	3.298715	2.756715
C	-2.768901	-1.324327	-1.055865
C	-3.864525	-1.825398	-0.330564
C	-2.422948	-1.933121	-2.275420
C	-4.596540	-2.912188	-0.816035
H	-4.156435	-1.358799	0.613198
C	-3.159325	-3.018682	-2.757794
H	-1.574566	-1.571097	-2.860390
C	-4.244825	-3.514019	-2.028496
H	-5.449459	-3.287316	-0.245047
H	-2.882746	-3.479476	-3.709370
H	-4.818026	-4.363739	-2.406703
C	3.218328	0.271321	-1.196670
C	4.315468	0.472870	-0.317857
C	3.436473	-0.240274	-2.488354
C	5.598685	0.154470	-0.787607
C	4.724153	-0.551706	-2.927740
C	5.808159	-0.350508	-2.072677
H	6.459670	0.303360	-0.133960
H	4.875200	-0.947706	-3.934662
H	6.822232	-0.587754	-2.403691
C	1.443483	2.377129	-0.198489
C	0.502783	2.851995	0.728829
C	2.274166	3.294669	-0.864663
C	0.386167	4.221527	0.982358
H	-0.151778	2.156709	1.252883
C	2.162087	4.662202	-0.601723
H	3.017026	2.941714	-1.584114
C	1.217757	5.128518	0.319855
H	-0.355984	4.575947	1.701766
H	2.816329	5.367595	-1.120038
H	1.132741	6.199086	0.521942
C	-0.888684	-2.634552	1.897864
C	-0.570914	-3.267228	0.538052
C	0.170523	-4.606811	0.558440
C	1.560330	-4.594492	1.199776
C	2.494767	-3.506011	0.653572
C	2.281027	-2.124343	1.276411
H	-0.801998	-3.396063	2.679188
H	-1.905676	-2.223367	1.909257
H	-1.520533	-3.377447	-0.005511
H	-0.008887	-2.601173	-0.191985
H	-0.473092	-5.342513	1.070341
H	0.260589	-4.952386	-0.486206
H	2.009315	-5.589708	1.046554
H	1.470987	-4.471428	2.294470
H	3.539201	-3.817825	0.843878
H	2.409022	-3.460522	-0.449976
H	2.416310	-2.203266	2.369801
H	3.061657	-1.440439	0.916603
C	0.628423	-0.155499	2.822250
C	-0.024540	-1.334697	3.288078
H	0.066972	0.783637	2.831408
H	1.698898	-0.045974	3.019866
H	0.591640	-2.096221	3.771671
H	-1.022858	-1.240186	3.724041
H	2.602662	-0.403306	-3.172216
C	4.126040	1.041023	1.077775
C	5.085974	0.519797	2.148369
H	3.094508	0.846031	1.410113
H	4.197405	2.141938	1.018838
H	5.062041	-0.580158	2.204882
H	6.127033	0.827172	1.965375
H	4.802689	0.917750	3.135491
C	-4.234379	1.814695	-1.540196
C	-3.811846	3.117561	-2.234337
H	-5.317962	1.669849	-1.685810
H	-3.756584	0.953818	-2.025483
H	-4.360376	3.981010	-1.825882
H	-2.737900	3.320709	-2.101393
H	-4.018833	3.069290	-3.315339

^{4}TS9-10C-10
Geometry with 89 atoms:
Total energy: -3202.740823620

Cr	0.259923	0.248375	1.322350
P	-1.548968	0.295547	-0.639205
P	1.803856	0.387140	-0.688971
C	0.743392	0.283876	-2.211275
C	-0.555799	1.073670	-2.012351
H	1.304091	0.632407	-3.091447
H	0.535272	-0.783694	-2.382647
H	-0.328221	2.112517	-1.733937
H	-1.151012	1.102457	-2.937502
C	-3.013257	1.393084	-0.409132
C	-2.968283	2.719428	-0.883843
C	-4.144458	0.958639	0.329340
C	-4.015602	3.610204	-0.646903
H	-2.108094	3.077345	-1.450226
C	-5.185348	1.875646	0.551606
C	-5.131925	3.185586	0.076055
H	-3.955695	4.632364	-1.027961
H	-6.059821	1.546196	1.120140
H	-5.958156	3.873225	0.272175
C	-2.183167	-1.204773	-1.502174
C	-1.919994	-2.483330	-0.989451
C	-2.924817	-1.083036	-2.690348
C	-2.386014	-3.623616	-1.651903
H	-1.356307	-2.595198	-0.062346
C	-3.385032	-2.221678	-3.354430
H	-3.158451	-0.093860	-3.092851
C	-3.116294	-3.494039	-2.836173
H	-2.177513	-4.614257	-1.240455
H	-3.962128	-2.116050	-4.276286
H	-3.480804	-4.383907	-3.355097
C	3.152034	-0.843878	-0.954615
C	2.902169	-2.232620	-0.799091
C	4.442419	-0.401785	-1.299141
C	3.972377	-3.122139	-0.980742
C	5.487611	-1.308066	-1.480246
C	5.251139	-2.673398	-1.315962
H	3.803833	-4.193899	-0.862532
H	6.482643	-0.943699	-1.746242
H	6.061854	-3.393950	-1.449435
C	2.623070	2.031780	-0.789181
C	3.426304	2.446154	0.291274
C	2.456543	2.903653	-1.878048
C	4.048048	3.695302	0.278033
H	3.575689	1.786905	1.147827
C	3.072767	4.159932	-1.883004
H	1.853407	2.619386	-2.741508
C	3.868971	4.559310	-0.807757
H	4.673021	3.995733	1.122527
H	2.931323	4.825257	-2.738270
H	4.351401	5.539627	-0.815330
C	-1.326968	0.026744	2.854164
C	-0.890838	-1.421771	2.594549
C	-0.307007	-2.161372	3.804342
C	0.928543	-1.512469	4.433634
C	2.068768	-1.240133	3.443468
C	1.910963	0.028242	2.596147
H	-1.341598	0.211393	3.932442
H	-2.319839	0.213426	2.440756
H	-1.756803	-1.975499	2.197922
H	-0.145652	-1.575125	1.751177
H	-1.104909	-2.257550	4.560236
H	-0.054164	-3.188536	3.488622
H	1.283322	-2.179350	5.236710
H	0.649589	-0.567059	4.932979
H	3.011642	-1.165511	4.017581
H	2.201736	-2.125843	2.793610
H	1.893977	0.912406	3.260876
H	2.812127	0.132182	1.969472
C	0.109898	2.322381	1.493045
C	-0.664354	1.982814	2.638184
H	-0.406341	2.775591	0.638898
H	1.132597	2.675734	1.648162
H	-0.170856	2.039172	3.611158
H	-1.717233	2.273693	2.658355
H	4.640785	0.663262	-1.425711
C	1.516325	-2.764349	-0.493759
C	1.441451	-4.024289	0.368638
H	0.984564	-2.944296	-1.445354
H	0.936261	-1.967650	0.000385
H	1.839081	-4.908646	-0.151467
H	2.005605	-3.904067	1.306461
H	0.394455	-4.251635	0.625662
C	-4.316460	-0.446976	0.874781
C	-5.315662	-1.296400	0.078413
H	-4.662750	-0.373295	1.919637
H	-3.351052	-0.970444	0.912985
H	-4.991253	-1.420939	-0.964523
H	-5.417893	-2.297943	0.525661
H	-6.312277	-0.827643	0.068100

^{4}TS9-10C-11
Geometry with 89 atoms:
Total energy: -3202.739973580

Cr	0.195249	0.009232	1.358218
P	-1.569999	0.213780	-0.700738
P	1.764338	0.534678	-0.546066
C	0.819318	0.345467	-2.135914
C	-0.542989	1.039234	-2.022122
H	1.405394	0.734701	-2.981400
H	0.698580	-0.732284	-2.319625
H	-0.406365	2.095372	-1.747911
H	-1.087440	1.010051	-2.978306
C	-3.027112	1.314912	-0.465335
C	-3.030741	2.623100	-0.982036
C	-4.126918	0.865332	0.314607
C	-4.095868	3.492157	-0.736324
H	-2.198923	2.986082	-1.586350
C	-5.182898	1.758732	0.547749
C	-5.174582	3.057438	0.033108
H	-4.077034	4.504520	-1.146503
H	-6.035897	1.434801	1.146124
H	-6.013631	3.727549	0.235674
C	-2.221541	-1.239966	-1.625405
C	-1.698787	-2.518519	-1.381325
C	-3.223532	-1.083690	-2.599798
C	-2.161588	-3.624515	-2.101883
H	-0.928363	-2.657301	-0.622928
C	-3.687740	-2.189525	-3.314758
H	-3.651884	-0.096596	-2.792464
C	-3.157154	-3.461637	-3.068205
H	-1.746151	-4.615415	-1.902922
H	-4.469576	-2.059228	-4.067202
H	-3.523928	-4.325469	-3.627945
C	3.327929	-0.426390	-0.749166
C	3.325148	-1.843297	-0.760369
C	4.554058	0.263191	-0.822116
C	4.558420	-2.511938	-0.830517
C	5.764552	-0.424913	-0.898986
C	5.767678	-1.821338	-0.896787
H	4.562671	-3.605709	-0.829224
H	6.702361	0.132684	-0.955281
H	6.709964	-2.372506	-0.945328
C	2.289352	2.299656	-0.535340
C	2.746148	2.861842	0.671343
C	2.268900	3.101233	-1.689776
C	3.171012	4.190887	0.719768
H	2.782764	2.258008	1.578968
C	2.684736	4.435153	-1.635230
H	1.936449	2.698977	-2.647859
C	3.137040	4.983040	-0.432270
H	3.527939	4.609467	1.663826
H	2.660027	5.044797	-2.541835
H	3.464875	6.024599	-0.392411
C	-1.164636	-0.783864	2.932387
C	-0.709866	-2.031208	2.162395
C	0.040247	-3.073827	3.008270
C	1.261996	-2.550903	3.777922
C	2.252849	-1.705895	2.963438

C	1.804859	-0.270010	2.654872
H	-0.709846	-0.759104	3.925348
H	-2.252178	-0.792020	3.034517
H	-1.576561	-2.489926	1.664108
H	-0.020974	-1.862123	1.273443
H	-0.675353	-3.522475	3.717455
H	0.355010	-3.888658	2.332715
H	1.785596	-3.427394	4.194214
H	0.933702	-1.964773	4.654319
H	3.199477	-1.665639	3.534885
H	2.512469	-2.238812	2.030528
H	1.530911	0.248520	3.593381
H	2.661675	0.282064	2.234113
C	-0.273791	1.943197	1.941833
C	-1.261196	1.269581	2.722165
H	-0.612061	2.500581	1.060734
H	0.580566	2.385579	2.461703
H	-1.190302	1.329261	3.810717
H	-2.288709	1.292259	2.350255
H	4.569142	1.353419	-0.816522
C	2.067290	-2.687183	-0.739880
C	1.754065	-3.351705	-2.086961
H	1.208193	-2.079220	-0.416752
H	2.178838	-3.472132	0.026699
H	2.582480	-4.004328	-2.403392
H	0.844237	-3.967600	-2.023139
H	1.602714	-2.607547	-2.884750
C	-4.179840	-0.549703	0.859338
C	-4.980675	-0.751193	2.146058
H	-3.150297	-0.903322	1.021021
H	-4.578156	-1.212550	0.070622
H	-4.655200	-0.060318	2.940847
H	-6.059776	-0.596349	1.994049
H	-4.853369	-1.780520	2.516104

^{4}TS9-10C-12
Geometry with 89 atoms:
Total energy: -3202.736679580

Cr	-0.479772	-1.085197	1.081573
P	1.557334	-0.266190	-0.521333
P	-1.696868	-0.171489	-0.935488
C	-0.559866	-0.568234	-2.353081
C	0.783273	0.147999	-2.179361
H	-0.413287	-1.659027	-2.349221
H	-1.025881	-0.305099	-3.314407
H	1.476361	-0.156781	-2.975746
H	0.656001	1.237057	-2.265704
C	3.027323	-1.294175	-0.948332
C	3.024187	-2.613446	-0.456568
C	4.106964	-0.850646	-1.756643
C	4.063463	-3.500296	-0.737111
H	2.189775	-2.953378	0.153410
C	5.138829	-1.766116	-2.027486
C	5.128855	-3.069434	-1.529409
H	4.036731	-4.519012	-0.343459
H	5.973098	-1.442323	-2.655971
H	5.951293	-3.748970	-1.766303
C	2.246120	1.296147	0.163420
C	3.274552	1.201458	1.119808
C	1.702387	2.559196	-0.124196
C	3.746461	2.344064	1.770382
H	3.722774	0.230774	1.347580
C	2.180216	3.701003	0.526414
H	0.895916	2.670971	-0.851572
C	3.199892	3.597906	1.476741
H	4.550797	2.254702	2.504831
H	1.749858	4.676032	0.284985
H	3.571054	4.491471	1.984103
C	-2.091998	1.614362	-1.220872
C	-1.935904	2.619490	-0.233285
C	-2.558083	1.959326	-2.503310
C	-2.225982	3.945986	-0.595365
C	-2.842915	3.282485	-2.837800
C	-2.666722	4.279939	-1.877515
H	-2.112346	4.741447	0.141655
H	-3.204522	3.528741	-3.838760
H	-2.882840	5.323254	-2.120889
C	-3.266985	-1.037783	-1.311916
C	-3.268900	-2.307592	-1.915470
C	-4.488593	-0.469234	-0.908963
C	-4.472481	-2.988615	-2.119472
H	-2.337466	-2.777249	-2.236820
C	-5.687534	-1.156557	-1.111514
H	-4.508985	0.520621	-0.446852
C	-5.682900	-2.417127	-1.716776
H	-4.461805	-3.971244	-2.597444
H	-6.630094	-0.701411	-0.797792
H	-6.622043	-2.952026	-1.877425
C	0.942690	-1.734675	2.641122
C	0.628340	-0.298758	3.062944
C	-0.038080	-0.151806	4.434530
C	-1.369511	-0.891834	4.598087
C	-2.424257	-0.527166	3.543883
C	-2.269345	-1.229642	2.188625
H	0.893864	-2.394098	3.512839
H	1.935302	-1.815059	2.184294
H	1.557433	0.291356	3.020197
H	-0.009106	0.296105	2.340796
H	0.678437	-0.499864	5.197996
H	-0.196108	0.923557	4.627828
H	-1.756632	-0.665350	5.605211
H	-1.201634	-1.984101	4.581790
H	-3.421042	-0.777409	3.953839
H	-2.436580	0.571780	3.419755
H	-2.424998	-2.313721	2.335737
H	-3.083368	-0.907719	1.517586
C	-0.617022	-3.045546	0.366224
C	0.002129	-3.328712	1.614069
H	-0.027784	-3.189895	-0.546209
H	-1.690268	-3.232295	0.266270
H	-0.638302	-3.638856	2.442343
H	0.986559	-3.802691	1.628342
H	-2.719473	1.180463	-3.252377
C	-1.475492	2.282372	1.171883
C	-1.442903	3.419206	2.188009
H	-0.460333	1.861040	1.099752
H	-2.113775	1.473316	1.557683
H	-0.740350	4.214278	1.893224
H	-2.436204	3.873589	2.329785
H	-1.110999	3.037547	3.166059
C	4.230971	0.540503	-2.351583
C	5.403090	1.351738	-1.782646
H	3.307039	1.114779	-2.214010
H	4.365246	0.433617	-3.442163
H	5.455658	2.340953	-2.264395
H	5.288016	1.509319	-0.700096
H	6.366927	0.845992	-1.950515

^{4}TS9-10C-13
Geometry with 89 atoms:
Total energy: -3202.739798060

Cr	0.194487	-0.021819	1.314458
P	-1.576736	0.266165	-0.708687
P	1.757675	0.617140	-0.570065
C	0.794455	0.552630	-2.159360
C	-0.579139	1.206352	-1.974911
H	1.366864	1.027214	-2.970419
H	0.690302	-0.506545	-2.438229
H	-0.460315	2.240580	-1.620099
H	-1.134077	1.241147	-2.925033
C	-3.073820	1.300189	-0.424006
C	-3.122271	2.632323	-0.872542
C	-4.162792	0.770659	0.319712
C	-4.222143	3.446990	-0.595434
H	-2.299687	3.056834	-1.448072
C	-5.255298	1.609675	0.584247
C	-5.291722	2.932474	0.136696
H	-4.237836	4.479082	-0.953131
H	-6.102523	1.223056	1.152857
H	-6.158627	3.558445	0.361990
C	-2.167665	-1.156975	-1.719307
C	-1.616966	-2.433335	-1.527645
C	-3.147913	-0.976331	-2.711075
C	-2.028648	-3.510786	-2.318968
H	-0.866761	-2.595627	-0.754006
C	-3.561582	-2.054026	-3.496782
H	-3.597149	0.008258	-2.864734
C	-3.001504	-3.322522	-3.303912
H	-1.591050	-4.499656	-2.161096
H	-4.326399	-1.904153	-4.262917
H	-3.327963	-4.164159	-3.919664
C	3.305266	-0.336831	-0.881300
C	3.274844	-1.752340	-1.000269
C	4.532733	0.343829	-0.961800
C	4.491238	-2.426472	-1.182403
C	5.728473	-0.351125	-1.150310
C	5.706374	-1.741339	-1.257250
H	4.495300	-3.513806	-1.270539
H	6.671611	0.197056	-1.209472
H	6.635519	-2.298618	-1.399632
C	2.288231	2.375381	-0.428824
C	2.818931	2.822927	0.795909
C	2.179454	3.290023	-1.490320
C	3.232737	4.146972	0.951188
H	2.920415	2.134548	1.635593
C	2.583382	4.619078	-1.327661
H	1.783160	2.983064	-2.459009
C	3.111286	5.051244	-0.108791
H	3.648432	4.473561	1.907452
H	2.488785	5.316888	-2.163331
H	3.428985	6.089343	0.015083
C	-1.160132	-0.856099	2.883053
C	-0.725276	-2.085143	2.074515
C	0.023195	-3.161616	2.878086
C	1.265057	-2.678022	3.640876
C	2.248341	-1.814616	2.836643
C	1.810338	-0.363826	2.588568
H	-0.695317	-0.863919	3.871780
H	-2.246831	-0.856424	2.995463
H	-1.598175	-2.522498	1.567619
H	-0.041518	-1.892907	1.189295
H	-0.686812	-3.621549	3.585604
H	0.316260	-3.958973	2.173159
H	1.787567	-3.573686	4.015697
H	0.960929	-2.119017	4.543147
H	3.206734	-1.805250	3.389444
H	2.483217	-2.314817	1.878935
H	1.551596	0.122825	3.548170
H	2.670213	0.191617	2.180561
C	-0.256987	1.895095	1.964708
C	-1.238289	1.206003	2.739343
H	-0.604965	2.485756	1.109457
H	0.612550	2.310576	2.481789
H	-1.148212	1.228821	3.827778
H	-2.271861	1.251217	2.385828
H	4.562920	1.430468	-0.873582
C	1.966315	-2.516582	-0.964474
C	2.033569	-3.988374	-0.561931
H	1.481526	-2.442893	-1.953872
H	1.285874	-1.985986	-0.276949
H	1.018042	-4.402783	-0.459290
H	2.551589	-4.598016	-1.317769
H	2.555432	-4.125489	0.397674
C	-4.165166	-0.670852	0.791735
C	-4.953286	-0.964474	2.068482
H	-3.123045	-0.993986	0.933222
H	-4.543018	-1.306956	-0.028498
H	-4.655017	-0.297390	2.893606
H	-6.038289	-0.848637	1.924721
H	-4.781848	-2.003494	2.390763

^{4}TS9-10C-14
Geometry with 89 atoms:
Total energy: -3202.737514760

Cr	-0.194338	-1.451122	0.472410
P	1.527017	0.144744	-0.775935
P	-1.672257	0.025294	-0.922914
C	-0.759915	0.094900	-2.540591
C	0.688409	0.592394	-2.407444
H	-0.796272	-0.941485	-2.908305
H	-1.318923	0.699917	-3.270911
H	1.288094	0.241777	-3.257110
H	0.715864	1.688679	-2.449655
C	3.123353	-0.678799	-1.218899
C	3.226153	-1.358732	-2.449981
C	4.192921	-0.776272	-0.289153
C	4.358891	-2.100492	-2.784358
H	2.413250	-1.322380	-3.176555
C	5.325546	-1.524427	-0.655245
C	5.420570	-2.180101	-1.881611
H	4.407087	-2.612949	-3.747994
H	6.153172	-1.597665	0.056032
H	6.315545	-2.756599	-2.127762

C	1.938389	1.822535	-0.146469
C	1.355543	2.276451	1.045655
C	2.756256	2.691972	-0.888508
C	1.588284	3.580028	1.493832
H	0.709603	1.615656	1.627225
C	2.983162	3.995311	-0.441878
H	3.222665	2.348625	-1.815977
C	2.399862	4.440671	0.749997
H	1.124656	3.925235	2.420669
H	3.621851	4.664709	-1.023450
H	2.578713	5.461126	1.097419
C	-1.845082	1.776909	-0.367729
C	-2.221181	2.069027	0.965725
C	-1.564801	2.836104	-1.253012
C	-2.257297	3.413006	1.372027
C	-1.610591	4.163149	-0.828056
C	-1.948086	4.452534	0.496309
H	-2.536535	3.642138	2.404236
H	-1.379533	4.967224	-1.530315
H	-1.975608	5.487904	0.844394
C	-3.354717	-0.518342	-1.407565
C	-3.559343	-1.866873	-1.751679
C	-4.437344	0.375284	-1.453583
C	-4.825417	-2.310336	-2.139276
H	-2.731237	-2.577432	-1.713110
C	-5.704523	-0.075898	-1.834958
H	-4.294472	1.425457	-1.192189
C	-5.901151	-1.416788	-2.176932
H	-4.973945	-3.360018	-2.404009
H	-6.541066	0.626643	-1.864603
H	-6.893390	-1.767162	-2.471584
C	1.427867	-2.302063	1.707134
C	0.787834	-1.247410	2.619492
C	0.190103	-1.791436	3.923986
C	-0.866272	-2.888667	3.757590
C	-2.040487	-2.507466	2.846451
C	-1.751504	-2.565373	1.339935
H	1.513707	-3.247983	2.248838
H	2.418651	-1.985080	1.379017
H	1.540335	-0.472756	2.836681
H	-0.031989	-0.608742	2.154280
H	1.022407	-2.168617	4.542176
H	-0.249209	-0.945950	4.481645
H	-1.244180	-3.140067	4.762493
H	-0.397810	-3.814449	3.377784
H	-2.880781	-3.191922	3.069695
H	-2.405859	-1.506993	3.140577
H	-1.535420	-3.614301	1.064884
H	-2.666094	-2.292697	0.787069
C	0.179288	-2.876756	-1.005183
C	1.012729	-3.428375	0.012299
H	0.673987	-2.457552	-1.886590
H	-0.775093	-3.372844	-1.205019
H	0.632349	-4.289763	0.565152
H	2.089948	-3.456857	-0.169012
H	-1.309174	2.638313	-2.294171
C	-2.630957	1.004971	1.959746
C	-4.134607	0.999873	2.266195
H	-2.070753	1.154419	2.899160
H	-2.348969	0.011700	1.586456
H	-4.461755	1.963463	2.687565
H	-4.723183	0.811506	1.355602
H	-4.377818	0.210776	2.995158
C	4.208905	-0.126803	1.083730
C	5.150970	1.079358	1.185428
H	4.528710	-0.886851	1.816865
H	3.197908	0.175691	1.387258
H	6.189534	0.790956	0.958661
H	4.861169	1.873338	0.483112
H	5.131975	1.501814	2.202581

^{4}TS9-10C-15
Geometry with 89 atoms:
Total energy: -3202.739646600

Cr	0.057177	-0.836500	1.143675
P	-1.706220	-0.219988	-0.481907
P	1.570677	0.264217	-0.782105
C	0.345322	0.657095	-2.138054
C	-0.875030	-0.269659	-2.148005
H	0.031803	1.693469	-1.936845
H	0.851398	0.672284	-3.115534
H	-1.576979	0.022672	-2.942286
H	-0.582511	-1.314638	-2.334206
C	-2.374101	1.489418	-0.336686
C	-1.811734	2.266720	0.695542
C	-3.324659	2.074297	-1.212128
C	-2.155835	3.604910	0.876709
H	-1.086405	1.808874	1.371241
C	-3.646125	3.429445	-1.015865
C	-3.077219	4.190245	0.005596
H	-1.705807	4.183825	1.686411
H	-4.365522	3.899526	-1.691923
H	-3.354733	5.240944	0.120835
C	-3.126839	-1.366484	-0.551396
C	-3.081786	-2.545298	-1.314678
C	-4.240328	-1.122024	0.271901
C	-4.144881	-3.451847	-1.269524
H	-2.222847	-2.768996	-1.950302
C	-5.297719	-2.033238	0.315306
H	-4.285237	-0.213174	0.876953
C	-5.254126	-3.198050	-0.457260
H	-4.104372	-4.361960	-1.872918
H	-6.160424	-1.829484	0.954178
H	-6.083081	-3.909147	-0.424362
C	2.780932	-0.908775	-1.527834
C	3.984986	-1.228769	-0.844128
C	2.467409	-1.573185	-2.727149
C	4.823380	-2.205359	-1.403549
C	3.317248	-2.544044	-3.260614
C	4.500773	-2.860185	-2.594247
H	5.754450	-2.464442	-0.897368
H	3.051677	-3.047898	-4.192921
H	5.177148	-3.617095	-2.998746
C	2.443593	1.875061	-0.636071
C	1.979332	2.813658	0.300932
C	3.520921	2.214054	-1.471536
C	2.582380	4.070501	0.401154
H	1.135443	2.571958	0.950727
C	4.125711	3.469079	-1.364119
H	3.894374	1.493772	-2.203575
C	3.658875	4.398426	-0.428424
H	2.210859	4.794147	1.130882
H	4.965195	3.722764	-2.016182
H	4.134567	5.378696	-0.346164
C	1.625741	-1.268736	2.667483
C	1.279260	0.216451	2.866036
C	0.739807	0.580240	4.259696
C	-0.484024	-0.219960	4.731710
C	-1.624125	-0.373918	3.711874
C	-1.355768	-1.372978	2.576765
H	1.263676	-1.856537	3.513666
H	2.708863	-1.382378	2.587745
H	2.152867	0.836361	2.614115
H	0.504813	0.662216	2.163028
H	1.558056	0.463894	4.989977
H	0.491319	1.656238	4.247737
H	-0.867382	0.274326	5.639641
H	-0.171189	-1.227454	5.058448
H	-2.520858	-0.701199	4.271812
H	-1.895181	0.620307	3.305445
H	-1.013080	-2.334997	3.001734
H	-2.293903	-1.596593	2.045335
C	0.289634	-2.733121	0.363850
C	1.379435	-2.769299	1.294964
H	0.552604	-2.675949	-0.698892
H	-0.605839	-3.321265	0.589940
H	1.318661	-3.473868	2.127644
H	2.383274	-2.685511	0.871568
H	1.548714	-1.341887	-3.267089
C	4.383555	-0.519233	0.437035
C	5.270010	-1.310612	1.398976
H	3.472224	-0.202257	0.966314
H	4.888973	0.425681	0.171008
H	4.837161	-2.295511	1.638802
H	6.277005	-1.483216	0.989415
H	5.398282	-0.756041	2.341586
C	-4.032464	1.338237	-2.334730
C	-5.546767	1.207729	-2.118701
H	-3.613862	0.334397	-2.473805
H	-3.848239	1.884267	-3.276409
H	-6.011382	0.678179	-2.965421
H	-5.768725	0.638994	-1.203298
H	-6.033589	2.191508	-2.030973

^{4}TS9-10C-16
Geometry with 89 atoms:
Total energy: -3202.735261360

Cr	-0.090605	-0.288344	1.490118
P	1.712844	-0.314851	-0.449082
P	-1.580242	-0.307943	-0.543189
C	-0.620699	-0.488221	-2.141915
C	0.828318	-0.953095	-1.964074
H	-1.154031	-1.172795	-2.817594
H	-0.659882	0.501090	-2.618490
H	0.861333	-2.044855	-1.810269
H	1.410936	-0.746562	-2.874105
C	3.291876	-1.262634	-0.490149
C	3.459775	-2.203680	0.545215
C	4.274805	-1.161541	-1.509640
C	4.571246	-3.043792	0.596780
H	2.702250	-2.283321	1.322884
C	5.382432	-2.024829	-1.435741
C	5.538190	-2.952641	-0.406040
H	4.676470	-3.765172	1.410379
H	6.142188	-1.970379	-2.219960
H	6.413552	-3.606775	-0.390823
C	2.159299	1.450914	-0.689441
C	3.313143	1.947686	-0.053509
C	1.302256	2.357533	-1.338086
C	3.605050	3.313646	-0.077302
H	3.997483	1.263243	0.453713
C	1.599845	3.723470	-1.361444
H	0.393258	2.015335	-1.831695
C	2.749660	4.206630	-0.730927
H	4.509651	3.680421	0.414115
H	0.923980	4.411380	-1.875331
H	2.979767	5.274493	-0.749860
C	-2.645503	1.162005	-0.829246
C	-3.614146	1.274036	-1.859311
C	-2.376464	2.268559	-0.000479
C	-4.273995	2.507641	-2.001671
C	-3.044857	3.480558	-0.163678
C	-4.001781	3.597320	-1.174231
H	-5.018151	2.615392	-2.795264
H	-2.818868	4.323491	0.493325
H	-4.535154	4.539563	-1.322930
C	-2.657519	-1.784865	-0.441291
C	-3.907094	-1.710253	0.195846
C	-2.190337	-3.030332	-0.895689
C	-4.680112	-2.862354	0.363837
H	-4.287468	-0.749127	0.548448
C	-2.968036	-4.178473	-0.727371
H	-1.214825	-3.115407	-1.381740
C	-4.214058	-4.097278	-0.096973
H	-5.654514	-2.791299	0.853225
H	-2.597783	-5.140680	-1.089437
H	-4.821000	-4.996232	0.034374
C	1.487704	-0.072973	3.020475
C	1.090696	1.378420	2.725936
C	0.515696	2.152573	3.917181
C	-0.738665	1.545278	4.551848
C	-1.891999	1.318946	3.564693
C	-1.778227	0.056035	2.701425
H	1.555054	-0.215401	4.103374
H	2.450236	-0.324510	2.562465
H	1.967918	1.900609	2.312707
H	0.359198	1.530530	1.868349
H	1.311910	2.243717	4.675707
H	0.289986	3.179995	3.582225
H	-1.066933	2.222302	5.357829
H	-0.490586	0.589788	5.048976
H	-2.834202	1.266334	4.142562
H	-1.999500	2.219886	2.932138
H	-1.836863	-0.828081	3.361457
H	-2.667612	-0.008301	2.053655
C	-0.112543	-2.342921	1.809778
C	0.623583	-1.964946	2.971758
H	0.413540	-2.891867	1.021055
H	-1.169002	-2.602177	1.924396
H	0.073225	-1.879849	3.911485
H	1.636330	-2.353715	3.106255
H	-1.630233	2.175762	0.789578
C	-3.978113	0.160030	-2.824251

C	-5.441323	-0.291482	-2.726168
H	-3.333018	-0.714076	-2.674811
H	-3.779993	0.516382	-3.850422
H	-5.671761	-0.673604	-1.720390
H	-6.139256	0.532166	-2.942991
H	-5.643322	-1.098555	-3.448016
C	4.217654	-0.194127	-2.679045
C	5.388243	0.797196	-2.722550
H	3.281775	0.376648	-2.671788
H	4.212141	-0.785048	-3.611903
H	5.412369	1.422405	-1.817344
H	6.358946	0.283941	-2.803785
H	5.291949	1.466850	-3.591805

^{4}TS9-10C-17
Geometry with 89 atoms:
Total energy: -3202.739233590

Cr	-0.094989	-0.049908	1.536139
P	1.665897	-0.209002	-0.697596
P	-1.674241	-0.547262	-0.336127
C	-0.696023	-1.393717	-1.667531
C	0.463704	-0.497447	-2.112699
H	-0.312462	-2.330104	-1.231413
H	-1.337357	-1.671376	-2.514373
H	1.002420	-0.960737	-2.950940
H	0.089400	0.474120	-2.468868
C	3.120637	-1.234785	-1.215066
C	3.659246	-0.966945	-2.493216
C	3.681674	-2.261353	-0.425696
C	4.723640	-1.706304	-2.998346
H	3.242091	-0.157130	-3.097408
C	4.751262	-3.005183	-0.963043
C	5.268455	-2.740640	-2.227569
H	5.126394	-1.479784	-3.988389
H	5.183877	-3.809916	-0.362384
H	6.098561	-3.336920	-2.614414
C	2.278735	1.512824	-0.921748
C	1.392742	2.554285	-1.250015
C	3.606729	1.833497	-0.586197
C	1.825278	3.883232	-1.244583
H	0.352276	2.345202	-1.506619
C	4.034799	3.164150	-0.579724
H	4.315571	1.041239	-0.334182
C	3.145942	4.193489	-0.905651
H	1.123545	4.678464	-1.508706
H	5.071205	3.395909	-0.321719
H	3.483008	5.232747	-0.900592
C	-2.448449	0.934687	-1.105379
C	-3.314066	0.925574	-2.228340
C	-2.135002	2.159204	-0.482488
C	-3.822375	2.158473	-2.674294
C	-2.646053	3.369727	-0.947203
C	-3.499088	3.365215	-2.053133
H	-4.497018	2.164408	-3.535088
H	-2.387533	4.303547	-0.442667
H	-3.919990	4.300903	-2.429388
C	-3.030835	-1.688283	0.117581
C	-4.294950	-1.179487	0.463875
C	-2.797437	-3.071472	0.218650
C	-5.308417	-2.041286	0.889959
H	-4.495057	-0.108270	0.390333
C	-3.816473	-3.928710	0.641463
H	-1.820925	-3.493778	-0.027115
C	-5.073371	-3.416662	0.978044
H	-6.288110	-1.634001	1.151342
H	-3.625210	-5.002526	0.708337
H	-5.868500	-4.089175	1.308718
C	1.597441	0.365799	2.893472
C	1.267614	1.760743	2.348907
C	0.790226	2.783938	3.383043
C	-0.467600	2.397705	4.165949
C	-1.677405	2.055723	3.285384
C	-1.688842	0.631722	2.720506
H	1.755330	0.424740	3.974846
H	2.496681	-0.038960	2.418747
H	2.158217	2.138094	1.822463
H	0.526947	1.793593	1.488569
H	1.622243	2.968061	4.084077
H	0.611865	3.739303	2.859562
H	-0.718857	3.239337	4.832169
H	-0.251686	1.543360	4.832612
H	-2.594354	2.195913	3.888587
H	-1.756072	2.804654	2.474638
H	-1.744059	-0.084277	3.559610
H	-2.611105	0.476057	2.136291
C	-0.205744	-1.995553	2.271246
C	0.642047	-1.456492	3.282419
H	0.227768	-2.714045	1.566353
H	-1.262261	-2.155686	2.503564
H	0.177712	-1.157147	4.225190
H	1.645409	-1.870953	3.404454
H	-1.482370	2.155957	0.391321
C	-3.701380	-0.317245	-3.003667
C	-2.996976	-0.408863	-4.365671
H	-4.791697	-0.299367	-3.167138
H	-3.507852	-1.223786	-2.415579
H	-1.900366	-0.416349	-4.257124
H	-3.292613	-1.326784	-4.898124
H	-3.254400	0.449750	-5.005536
C	3.235592	-2.575302	0.984999
C	4.275598	-2.170999	2.038591
H	3.035245	-3.656924	1.070243
H	2.288027	-2.065335	1.190770
H	4.499836	-1.093052	1.988030
H	3.919971	-2.399158	3.056260
H	5.225874	-2.707621	1.892221

^{4}TS9-10C-18
Geometry with 89 atoms:
Total energy: -3202.740640020

Cr	-0.524148	-0.801274	1.254292
P	1.518288	-0.306840	-0.486890
P	-1.758672	-0.237862	-0.868794
C	-0.622802	-0.791253	-2.234176
C	0.701263	-0.024249	-2.149851
H	-0.451066	-1.872281	-2.113948
H	-1.104748	-0.640295	-3.212307
H	1.381336	-0.351504	-2.948374
H	0.526769	1.051964	-2.294914
C	2.863035	-1.515829	-0.841510
C	2.763412	-2.760325	-0.191095
C	3.938693	-1.277707	-1.736877
C	3.698213	-3.773357	-0.403842
H	1.938158	-2.936943	0.495017
C	4.863617	-2.317076	-1.936984
C	4.755202	-3.547070	-1.287009
H	3.597770	-4.730396	0.113344
H	5.693357	-2.152333	-2.629969
H	5.496079	-4.328466	-1.473601
C	2.385525	1.246323	-0.017871
C	3.408745	1.154057	0.944965
C	1.998371	2.516635	-0.474982
C	4.030127	2.305255	1.434212
H	3.735420	0.175031	1.305628
C	2.628008	3.666419	0.012360
H	1.203463	2.629717	-1.214606
C	3.641687	3.566142	0.969084
H	4.827177	2.215719	2.176539
H	2.322167	4.646260	-0.362340
H	4.131407	4.466341	1.347722
C	-2.160293	1.490458	-1.389434
C	-1.857762	2.623131	-0.593712
C	-2.755088	1.657312	-2.653172
C	-2.148987	3.892839	-1.119859
C	-3.040539	2.927676	-3.152497
C	-2.729581	4.048677	-2.380651
H	-1.924848	4.784057	-0.532586
H	-3.504080	3.039004	-4.135438
H	-2.944061	5.052067	-2.756967
C	-3.320752	-1.159690	-1.112627
C	-3.330934	-2.454969	-1.658194
C	-4.528702	-0.596199	-0.662626
C	-4.529608	-3.168023	-1.757484
H	-2.410267	-2.920528	-2.014303
C	-5.722041	-1.314402	-0.761392
H	-4.543185	0.412969	-0.243694
C	-5.725760	-2.601675	-1.308589
H	-4.525806	-4.171516	-2.190065
H	-6.654008	-0.863516	-0.411981
H	-6.660939	-3.161231	-1.387444
C	0.919171	-1.346379	2.851904
C	0.728591	0.147061	3.119176
C	0.104655	0.491828	4.475318
C	-1.271681	-0.125310	4.739887
C	-2.323209	0.201345	3.670136
C	-2.275713	-0.675347	2.412654
H	0.855643	-1.900397	3.793540
H	1.881756	-1.558939	2.372319
H	1.701096	0.652275	3.003770
H	0.132518	0.704106	2.336109
H	0.810834	0.176808	5.262519
H	0.028073	1.590525	4.551701
H	-1.617021	0.235878	5.722641
H	-1.183593	-1.222146	4.839217
H	-3.324865	0.097744	4.128952
H	-2.240732	1.273185	3.407755
H	-2.509880	-1.716760	2.696870
H	-3.085333	-0.369511	1.728402
C	-0.815294	-2.841209	0.803745
C	-0.170184	-3.012710	2.053923
H	-0.272940	-3.133746	-0.101748
H	-1.901975	-2.957090	0.756953
H	-0.792274	-3.170199	2.937864
H	0.789694	-3.532136	2.098762
H	-3.009871	0.780688	-3.254414
C	-1.259147	2.468136	0.790497
C	-0.854472	3.738731	1.529417
H	-0.373479	1.816116	0.707092
H	-1.978973	1.910679	1.410333
H	-0.115141	4.326464	0.964535
H	-1.721333	4.384451	1.739587
H	-0.395644	3.479796	2.496469
C	4.172479	0.021836	-2.485609
C	5.431538	0.772038	-2.028813
H	3.312429	0.695407	-2.392403
H	4.264402	-0.212802	-3.560425
H	5.562427	1.696239	-2.613649
H	5.362489	1.050717	-0.966868
H	6.338248	0.160916	-2.159901

^{4}TS9-10C-19
Geometry with 89 atoms:
Total energy: -3202.739594880

Cr	0.266301	-0.368507	1.418447
P	-1.774168	-0.367856	-0.537663
P	1.308535	0.838875	-0.570221
C	0.461702	0.370730	-2.159793
C	-1.063231	0.457910	-2.057959
H	0.841967	0.993961	-2.983635
H	0.785601	-0.651854	-2.385335
H	-1.378907	1.508671	-1.995999
H	-1.547697	0.042057	-2.955525
C	-3.491452	0.326685	-0.490908
C	-4.594770	-0.474967	-0.839225
C	-3.700807	1.681689	-0.118703
C	-5.895423	0.026973	-0.796685
H	-4.445324	-1.506783	-1.156778
C	-5.021408	2.160074	-0.084276
C	-6.109715	1.350681	-0.410169
H	-6.735034	-0.616128	-1.071132
H	-5.202597	3.199089	0.197281
H	-7.122974	1.758075	-0.370438
C	-1.955611	-2.141565	-0.993689
C	-2.656727	-2.995746	-0.118694
C	-1.308079	-2.708955	-2.104570
C	-2.703000	-4.372069	-0.345401
H	-3.188120	-2.581002	0.741242
C	-1.345597	-4.090725	-2.323451
H	-0.769228	-2.087114	-2.819956
C	-2.038085	-4.926817	-1.444897
H	-3.259879	-5.014547	0.341055
H	-0.834820	-4.510961	-3.193454
H	-2.067462	-6.004934	-1.619180
C	3.112761	0.622705	-0.902100
C	3.675125	-0.646890	-1.187453
C	3.958260	1.743087	-0.783843
C	5.068518	-0.735540	-1.343309
C	5.338595	1.626755	-0.944707
C	5.898135	0.378407	-1.223890
H	5.510330	-1.713128	-1.556697
H	5.972529	2.511269	-0.848252
H	6.978737	0.270688	-1.345206
C	1.053308	2.655604	-0.431478

C	1.160647	3.253150	0.837260
C	0.764612	3.466935	-1.541853
C	0.978815	4.629253	0.992819
H	1.398192	2.642574	1.708804
C	0.570858	4.841933	-1.381529
H	0.690971	3.041676	-2.543793
C	0.676502	5.426177	-0.115682
H	1.070197	5.078050	1.984749
H	0.341271	5.459561	-2.253264
H	0.525680	6.501533	0.006020
C	-0.540190	-2.133923	2.518087
C	0.433199	-2.772329	1.525259
C	1.634222	-3.506050	2.130459
C	2.533800	-2.673477	3.049277
C	3.071192	-1.379574	2.421006
C	2.088681	-0.205515	2.436573
H	-0.384370	-2.562158	3.512918
H	-1.575366	-2.305574	2.210288
H	-0.144248	-3.451292	0.877530
H	0.849284	-2.071665	0.736528
H	1.251175	-4.381511	2.682158
H	2.239207	-3.908509	1.299543
H	3.376486	-3.314245	3.357755
H	1.993123	-2.425403	3.980757
H	3.982307	-1.081911	2.973688
H	3.419418	-1.584654	1.393527
H	1.823746	0.024464	3.484167
H	2.592341	0.694995	2.044300
C	-0.698506	0.886784	2.775076
C	-0.878202	-0.330996	3.493628
H	-1.582813	1.328811	2.312305
H	0.041577	1.600587	3.147382
H	-0.209064	-0.527651	4.334613
H	-1.897829	-0.690092	3.654977
H	3.535695	2.723532	-0.561315
C	2.872974	-1.922159	-1.361082
C	2.786136	-2.398975	-2.817119
H	1.859662	-1.803292	-0.952415
H	3.340195	-2.716812	-0.756736
H	3.787772	-2.604595	-3.225094
H	2.194764	-3.325623	-2.891461
H	2.322360	-1.640090	-3.467356
C	-2.558243	2.637081	0.173447
C	-2.791866	3.629744	1.315493
H	-2.330253	3.204685	-0.747307
H	-1.642657	2.066572	0.383934
H	-3.574301	4.364689	1.073200
H	-3.093344	3.116899	2.242923
H	-1.867821	4.191460	1.518688

^{4}TS9-10C-20
Geometry with 89 atoms:
Total energy: -3202.736156240

Cr	-0.399592	-1.390099	0.723180
P	1.656136	-0.025151	-0.396015
P	-1.582884	0.077914	-0.982693
C	-0.341611	0.158546	-2.367513
C	0.944244	0.847146	-1.895433
H	-0.131964	-0.880023	-2.665922
H	-0.761527	0.668283	-3.246802
H	1.695499	0.826079	-2.696305
H	0.759636	1.905419	-1.657306
C	3.223135	-0.784790	-0.998582
C	3.303403	-2.187734	-0.914672
C	4.320021	-0.051248	-1.521897
C	4.442210	-2.880864	-1.324119
H	2.457046	-2.745327	-0.519106
C	5.462214	-0.772551	-1.910904
C	5.532726	-2.162992	-1.818257
H	4.477837	-3.970245	-1.250355
H	6.322689	-0.220761	-2.299049
H	6.440410	-2.684416	-2.132275
C	2.175606	1.271175	0.800277
C	3.250939	1.004980	1.668687
C	1.445657	2.459731	0.967087
C	3.589688	1.913314	2.674551
H	3.838102	0.090556	1.552483
C	1.790085	3.366607	1.974202
H	0.600363	2.694743	0.318418
C	2.860155	3.096731	2.831829
H	4.432130	1.696275	3.336040
H	1.215985	4.290211	2.083767
H	3.128625	3.807077	3.617283
C	-2.034562	1.860288	-0.761687
C	-2.066265	2.526616	0.484337
C	-2.309497	2.586105	-1.941520
C	-2.300079	3.916763	0.486786
C	-2.558947	3.954376	-1.911574
C	-2.534464	4.628696	-0.685526
H	-2.304560	4.444780	1.444225
H	-2.768318	4.492771	-2.838818
H	-2.710620	5.706461	-0.644963
C	-3.084635	-0.679529	-1.709062
C	-2.990072	-1.733880	-2.634324
C	-4.354334	-0.264112	-1.270735
C	-4.146927	-2.350119	-3.119449
H	-2.018201	-2.082796	-2.987738
C	-5.506656	-0.887721	-1.754727
H	-4.447171	0.556401	-0.555419
C	-5.406335	-1.930575	-2.680657
H	-4.061813	-3.162577	-3.845374
H	-6.487653	-0.553015	-1.408738
H	-6.308651	-2.415317	-3.061050
C	1.003965	-2.413012	2.095268
C	0.571412	-1.191884	2.907091
C	-0.176049	-1.506249	4.207247
C	-1.442517	-2.354519	4.050111
C	-2.479404	-1.755558	3.090616
C	-2.212012	-1.986811	1.599993
H	0.958998	-3.308050	2.723157
H	2.019022	-2.298151	1.700824
H	1.461238	-0.574458	3.109782
H	-0.057715	-0.429210	2.349451
H	0.530525	-2.014264	4.885708
H	-0.439055	-0.551269	4.694581
H	-1.889174	-2.475176	5.050938
H	-1.180473	-3.375065	3.716519
H	-3.468399	-2.185434	3.339402
H	-2.576071	-0.678323	3.305168
H	-2.300004	-3.067190	1.386458
H	-3.008607	-1.505194	1.007908
C	-0.352512	-3.036218	-0.566412
C	0.230203	-3.657998	0.572559
H	0.286341	-2.860546	-1.438881
H	-1.402133	-3.249624	-0.789536
H	-0.421768	-4.247670	1.220530
H	1.244082	-4.059042	0.501958
H	-2.339552	2.069489	-2.903102
C	-1.914796	1.844256	1.826624
C	-3.208812	1.867881	2.651237
H	-1.108957	2.340343	2.392706
H	-1.596562	0.802002	1.685462
H	-3.583065	2.894795	2.783562
H	-4.004145	1.283087	2.162422
H	-3.044038	1.445293	3.653946
C	4.340901	1.454714	-1.706444
C	4.433610	1.889475	-3.175644
H	5.209423	1.857989	-1.157672
H	3.462575	1.919998	-1.242905
H	4.445942	2.988264	-3.253088
H	5.348797	1.510944	-3.656775
H	3.578244	1.518600	-3.763400

^{4}TS9-10C-21
Geometry with 89 atoms:
Total energy: -3202.738120980

Cr	-0.065207	-0.414989	1.338021
P	1.759403	-0.333648	-0.588806
P	-1.567153	-0.364442	-0.688376
C	-0.484296	-0.413769	-2.222433
C	0.808455	-1.188016	-1.944464
H	-1.052724	-0.889816	-3.034220
H	-0.248721	0.605515	-2.555713
H	0.583156	-2.215772	-1.618918
H	1.423822	-1.251780	-2.855608
C	3.300158	-1.314639	-0.378401
C	3.410115	-2.594778	-0.955261
C	4.348959	-0.824608	0.440096
C	4.539269	-3.386274	-0.740304
H	2.612772	-2.992102	-1.584231
C	5.474782	-1.639806	0.638070
C	5.577436	-2.905820	0.060539
H	4.604582	-4.375735	-1.198923
H	6.287950	-1.268507	1.268396
H	6.465301	-3.517313	0.238693
C	2.274930	1.208257	-1.449749
C	1.738017	2.444266	-1.058436
C	3.173832	1.161330	-2.529686
C	2.091843	3.616768	-1.734743
H	1.036745	2.498496	-0.224184
C	3.524988	2.332264	-3.204559
H	3.613677	0.208785	-2.836676
C	2.985670	3.561764	-2.807352
H	1.667861	4.573533	-1.420101
H	4.227132	2.286938	-4.040667
H	3.265489	4.477171	-3.334481
C	-2.525010	1.218772	-0.778000
C	-3.779002	1.414326	-0.142072
C	-1.876524	2.327136	-1.364555
C	-4.331062	2.709011	-0.156268
C	-2.444756	3.599227	-1.357504
C	-3.687109	3.792028	-0.749682
H	-5.296758	2.864333	0.332500
H	-1.915152	4.432304	-1.825843
H	-4.148486	4.782343	-0.730331
C	-2.708046	-1.760398	-1.031080
C	-2.700310	-2.897213	-0.209680
C	-3.556125	-1.721208	-2.151808
C	-3.532815	-3.981971	-0.503847
H	-2.049201	-2.932196	0.664101
C	-4.384044	-2.806493	-2.442655
H	-3.578577	-0.836552	-2.793749
C	-4.374572	-3.937869	-1.618254
H	-3.523513	-4.862734	0.142786
H	-5.044557	-2.766998	-3.312314
H	-5.026206	-4.784825	-1.846483
C	1.238757	0.202032	3.038237
C	0.681495	1.519986	2.466019
C	-0.150343	2.353876	3.455905
C	-1.337737	1.628883	4.106517
C	-2.244370	0.845662	3.144411
C	-1.668286	-0.491400	2.659059
H	0.827431	0.034676	4.036138
H	2.327157	0.265453	3.098984
H	1.513484	2.119308	2.067035
H	0.011840	1.452142	1.548991
H	0.524558	2.732293	4.241891
H	-0.519791	3.240495	2.912031
H	-1.934140	2.390301	4.635715
H	-0.977616	0.941906	4.892849
H	-3.201255	0.658276	3.667569
H	-2.509505	1.492530	2.287391
H	-1.320636	-1.085615	3.524806
H	-2.455512	-1.092714	2.175175
C	0.477033	-2.384522	1.653548
C	1.371732	-1.781050	2.601106
H	0.924257	-2.819386	0.752019
H	-0.372097	-2.946304	2.054871
H	1.211375	-2.001638	3.658719
H	2.428116	-1.752206	2.323772
H	-0.900565	2.213348	-1.834638
C	-4.582348	0.339906	0.566611
C	-5.890068	-0.018854	-0.150338
H	-4.818195	0.707904	1.578645
H	-3.987190	-0.567117	0.713728
H	-5.700856	-0.393335	-1.166859
H	-6.430636	-0.803222	0.402856
H	-6.556651	0.854200	-0.233234
C	4.326591	0.541865	1.097090
C	5.280479	1.553558	0.448737
H	4.599775	0.422432	2.159574
H	3.306767	0.954488	1.090066
H	5.020608	1.728428	-0.605317
H	5.238141	2.520290	0.975355
H	6.321462	1.195691	0.484184

^{4}TS9-10C-22
Geometry with 89 atoms:
Total energy: -3202.735939810

Cr	-0.099753	0.292181	1.541920
P	1.720888	-0.286989	-0.308800
P	-1.552241	-0.568880	-0.314597
C	-0.577597	-1.217924	-1.777420

C	0.909299	-1.470965	-1.504306
H	-1.059261	-2.131224	-2.156791
H	-0.696781	-0.456956	-2.561322
H	1.053384	-2.448172	-1.014364
H	1.460728	-1.508293	-2.454052
C	3.376119	-1.038919	-0.015044
C	3.622839	-1.448773	1.310502
C	4.377918	-1.233096	-1.001621
C	4.832901	-2.032281	1.683497
H	2.850601	-1.308334	2.064172
C	5.594670	-1.809151	-0.595607
C	5.829303	-2.205199	0.720986
H	4.996207	-2.342155	2.718229
H	6.380688	-1.949406	-1.342783
H	6.790155	-2.648809	0.993495
C	2.017329	1.321301	-1.152450
C	3.219073	2.021733	-0.937851
C	0.981948	1.959647	-1.861110
C	3.383626	3.317957	-1.433557
H	4.036687	1.552159	-0.386630
C	1.152076	3.255058	-2.357062
H	0.023607	1.466702	-2.025336
C	2.352308	3.939571	-2.144501
H	4.326361	3.843879	-1.263115
H	0.336446	3.730340	-2.907632
H	2.483379	4.953178	-2.530630
C	-2.748463	0.600766	-1.072395
C	-3.744536	0.240401	-2.014696
C	-2.595347	1.950090	-0.699262
C	-4.574295	1.261748	-2.510538
C	-3.418659	2.946474	-1.220764
C	-4.423097	2.594050	-2.125593
H	-5.358648	0.996993	-3.225102
H	-3.283118	3.985838	-0.913074
H	-5.090011	3.357463	-2.534021
C	-2.488735	-1.993917	0.351389
C	-3.773240	-1.819287	0.892789
C	-1.874210	-3.255418	0.428038
C	-4.433856	-2.895443	1.490942
H	-4.268302	-0.847413	0.833930
C	-2.540456	-4.328283	1.025047
H	-0.869198	-3.408663	0.027056
C	-3.820903	-4.150506	1.558859
H	-5.435888	-2.751866	1.902481
H	-2.055826	-5.306399	1.074644
H	-4.341034	-4.990085	2.026121
C	1.426765	1.242279	2.819052
C	0.892032	2.407735	1.971724
C	0.221146	3.535095	2.763505
C	-0.956199	3.111977	3.646560
C	-2.082452	2.392345	2.893023
C	-1.826525	0.911733	2.584007
H	1.492864	1.561803	3.863624
H	2.419639	0.934064	2.474611
H	1.726265	2.802623	1.371037
H	0.176179	2.133281	1.128921
H	0.996774	4.015511	3.384140
H	-0.119427	4.303379	2.047647
H	-1.354302	4.019806	4.129462
H	-0.600086	2.468917	4.471707
H	-3.004641	2.469393	3.499887
H	-2.307853	2.955360	1.968755
H	-1.785897	0.355785	3.537920
H	-2.700234	0.504743	2.048381
C	0.086011	-1.452358	2.636286
C	0.773868	-0.573399	3.532458
H	0.671903	-2.212065	2.107169
H	-0.936545	-1.752642	2.882430
H	0.210388	-0.192733	4.387710
H	1.818286	-0.787187	3.775524
H	-1.819038	2.220631	0.017813
C	-3.943205	-1.159374	-2.563146
C	-3.488012	-1.299956	-4.022932
H	-5.014841	-1.411765	-2.496035
H	-3.425880	-1.903301	-1.945052
H	-4.036772	-0.611864	-4.685042
H	-2.414708	-1.079251	-4.134532
H	-3.661895	-2.325490	-4.385841
C	4.223813	-0.896288	-2.472228
C	4.122002	-2.143116	-3.362875
H	5.098305	-0.301895	-2.786877
H	3.354860	-0.248838	-2.640600
H	5.025757	-2.768026	-3.288128
H	3.264898	-2.774110	-3.077664
H	3.998647	-1.857049	-4.419606

^{4}TS9-10C-23
Geometry with 89 atoms:
Total energy: -3202.734284640

Cr	-0.177191	-1.089092	-1.187547
P	1.839323	-0.005821	0.172938
P	-1.396796	0.476971	0.422206
C	-0.181306	0.984887	1.767770
C	1.052456	0.077505	1.854983
H	0.133033	2.007097	1.508433
H	-0.699721	1.048329	2.735576
H	1.760645	0.457446	2.606352
H	0.783305	-0.950499	2.145933
C	2.389411	1.723192	-0.145691
C	1.635502	2.414031	-1.115587
C	3.439755	2.396802	0.530462
C	1.907134	3.740675	-1.445651
H	0.809246	1.905292	-1.609846
C	3.711590	3.725035	0.157286
C	2.965671	4.395000	-0.812687
H	1.298509	4.252512	-2.194439
H	4.530734	4.249723	0.657214
H	3.208255	5.429614	-1.067954
C	3.328972	-1.052858	0.328475
C	4.285011	-0.999087	-0.702970
C	3.496262	-1.982207	1.369673
C	5.391171	-1.850305	-0.684981
H	4.170848	-0.277998	-1.517542
C	4.602912	-2.837881	1.378452
H	2.776436	-2.036759	2.189393
C	5.551231	-2.774512	0.353855
H	6.132303	-1.792355	-1.486046
H	4.726001	-3.552919	2.195629
H	6.416233	-3.441856	0.365376
C	-2.756416	-0.381646	1.336448
C	-4.083047	-0.493294	0.851336
C	-2.389055	-1.086833	2.502358
C	-4.990078	-1.278977	1.585804
C	-3.305006	-1.870501	3.202046
C	-4.620550	-1.962433	2.741947
H	-6.017076	-1.363276	1.219539
H	-2.990783	-2.403559	4.102485
H	-5.353553	-2.571399	3.276510
C	-2.006183	2.103989	-0.165159
C	-1.983121	2.402882	-1.536467
C	-2.441027	3.078484	0.748679
C	-2.392825	3.660341	-1.988835
H	-1.651513	1.649251	-2.254350
C	-2.842742	4.336421	0.293633
H	-2.472982	2.856263	1.818429
C	-2.819795	4.628259	-1.074540
H	-2.377046	3.883801	-3.058305
H	-3.180965	5.089558	1.009383
H	-3.137723	5.612078	-1.428302
C	1.051069	-2.908777	-1.546929
C	0.371767	-3.174739	-0.193144
C	-0.569229	-4.384203	-0.129107
C	-1.739370	-4.372015	-1.119005
C	-2.584326	-3.089288	-1.097037
C	-1.964392	-1.918361	-1.867744
H	0.898885	-3.774801	-2.197587
H	2.122873	-2.743647	-1.402359
H	1.167851	-3.274674	0.561440
H	-0.222567	-2.314831	0.254605
H	0.035776	-5.294360	-0.279690
H	-0.968454	-4.443354	0.898505
H	-2.375420	-5.242441	-0.887942
H	-1.366156	-4.539937	-2.145566
H	-3.573362	-3.324180	-1.534464
H	-2.796132	-2.807618	-0.049939
H	-1.777975	-2.238478	-2.909144
H	-2.682385	-1.084998	-1.937882
C	0.322624	-0.397744	-3.070958
C	0.861846	-1.721976	-3.190629
H	1.037971	0.429547	-3.034149
H	-0.608039	-0.181472	-3.606567
H	0.282294	-2.441190	-3.773222
H	1.940340	-1.819895	-3.339788
H	-1.368268	-1.035676	2.883587
C	-4.610136	0.171749	-0.404829
C	-5.516110	1.377004	-0.123688
H	-5.178573	-0.582831	-0.973549
H	-3.788876	0.479522	-1.061196
H	-6.392822	1.086226	0.476816
H	-4.976995	2.161513	0.427217
H	-5.881510	1.815500	-1.065873
C	4.249488	1.814175	1.671818
C	3.903545	2.448357	3.027346
H	5.320253	1.978203	1.463193
H	4.122049	0.727725	1.732039
H	4.503772	1.996153	3.833035
H	4.100792	3.531856	3.029157
H	2.838954	2.311847	3.279419

^{4}TS9-10C-24
Geometry with 89 atoms:
Total energy: -3202.737995160

Cr	0.091707	0.452996	1.305600
P	-1.791309	0.305456	-0.565635
P	1.536623	0.390259	-0.777981
C	0.393313	0.391465	-2.267804
C	-0.897721	1.157298	-1.961069
H	0.927458	0.850297	-3.112124
H	0.155849	-0.638715	-2.563456
H	-0.675169	2.191913	-1.656221
H	-1.542288	1.199922	-2.852999
C	-3.347441	1.252762	-0.321830
C	-3.505673	2.519972	-0.915223
C	-4.358274	0.750780	0.535990
C	-4.647723	3.286729	-0.679737
H	-2.735584	2.925283	-1.572419
C	-5.498370	1.540606	0.753746
C	-5.649765	2.793637	0.158711
H	-4.751605	4.266518	-1.151800
H	-6.282605	1.160292	1.414563
H	-6.547496	3.385564	0.352864
C	-2.294173	-1.261537	-1.388162
C	-3.236365	-1.254561	-2.431576
C	-1.701744	-2.475820	-1.008855
C	-3.575949	-2.442730	-3.081847
H	-3.718604	-0.319705	-2.728643
C	-2.043388	-3.665619	-1.660905
H	-0.966845	-2.501640	-0.202771
C	-2.981055	-3.650195	-2.696799
H	-4.311906	-2.427992	-3.889527
H	-1.575431	-4.604820	-1.355769
H	-3.251268	-4.579188	-3.204805
C	2.549510	-1.155549	-0.913638
C	3.848152	-1.284167	-0.344120
C	1.932802	-2.285581	-1.485441
C	4.468908	-2.542703	-0.412206
C	2.571515	-3.525002	-1.530523
C	3.851892	-3.651144	-0.994710
H	5.467120	-2.665092	0.009282
H	2.065637	-4.380651	-1.984034
H	4.372955	-4.611289	-1.021859
C	2.620754	1.813283	-1.185455
C	2.613479	2.961952	-0.382505
C	3.440961	1.769405	-2.326883
C	3.418720	4.056592	-0.715679
H	1.985986	3.000014	0.508420
C	4.245119	2.861732	-2.654015
H	3.463186	0.872339	-2.952065
C	4.235256	4.007198	-1.847990
H	3.409201	4.948218	-0.084075
H	4.885455	2.819075	-3.538521
H	4.867294	4.860769	-2.105081
C	-1.134543	-0.196635	3.052905
C	-0.554940	-1.497099	2.465542
C	0.343215	-2.301849	3.420396
C	1.529455	-1.537843	4.028116
C	2.370753	-0.713991	3.040534
C	1.720738	0.599351	2.586173
H	-0.694852	-0.010602	4.035340
H	-2.217676	-0.294380	3.151255
H	-1.380171	-2.124901	2.097009
H	0.076639	-1.406408	1.524250
H	-0.286754	-2.704603	4.231086

H	0.721378	-3.174448	2.860140
H	2.173003	-2.279866	4.528701
H	1.175037	-0.868333	4.831866
H	3.335288	-0.489179	3.533325
H	2.636020	-1.342570	2.169445
H	1.373545	1.171103	3.466684
H	2.461220	1.242765	2.082488
C	-0.501049	2.405547	1.631873
C	-1.348337	1.776102	2.606495
H	-0.990213	2.821214	0.743211
H	0.337958	2.998864	2.008178
H	-1.167354	2.007725	3.658484
H	-2.410216	1.709962	2.357823
H	0.928786	-2.219087	-1.902768
C	4.574275	-0.124660	0.316042
C	5.680558	-0.490434	1.305286
H	3.840396	0.509018	0.830003
H	4.996861	0.518513	-0.474431
H	5.320874	-1.184821	2.080651
H	6.549048	-0.953840	0.812010
H	6.043887	0.418429	1.809516
C	-4.279170	-0.602118	1.216629
C	-5.229122	-1.649439	0.621188
H	-4.519298	-0.468551	2.285369
H	-3.249599	-0.989280	1.183025
H	-6.277236	-1.318067	0.689395
H	-5.004183	-1.836354	-0.438818
H	-5.141834	-2.605424	1.161720

^{4}TS9-10C-25
Geometry with 89 atoms:
Total energy: -3202.737078790

Cr	-0.240411	-1.472828	0.445457
P	1.483719	0.105152	-0.809547
P	-1.716861	0.039531	-0.917284
C	-0.823947	0.051170	-2.548878
C	0.637607	0.518167	-2.446596
H	-0.885567	-0.990792	-2.893365
H	-1.377930	0.650725	-3.287211
H	1.217117	0.124728	-3.291321
H	0.690230	1.611126	-2.527290
C	3.089063	-0.708684	-1.234893
C	3.217380	-1.391756	-2.461377
C	4.146300	-0.789055	-0.289592
C	4.365433	-2.118071	-2.777575
H	2.413052	-1.370582	-3.197956
C	5.294984	-1.520751	-0.637522
C	5.416320	-2.178081	-1.860862
H	4.434046	-2.633494	-3.738406
H	6.113602	-1.580005	0.085410
H	6.323136	-2.741578	-2.093446
C	1.881988	1.797821	-0.210937
C	1.322945	2.251731	0.991785
C	2.666608	2.674769	-0.979640
C	1.541899	3.562731	1.424173
H	0.707499	1.582933	1.595932
C	2.881928	3.985264	-0.548507
H	3.116031	2.332344	-1.915879
C	2.319407	4.431093	0.653338
H	1.094466	3.906590	2.359538
H	3.494767	4.660518	-1.150724
H	2.488310	5.457668	0.987420
C	-1.885933	1.812663	-0.430903
C	-2.297719	2.177377	0.874361
C	-1.605624	2.821864	-1.373043
C	-2.390369	3.545291	1.184186
C	-1.691153	4.171526	-1.037520
C	-2.083075	4.535143	0.252411
H	-2.722343	3.840339	2.182444
H	-1.458389	4.933717	-1.784456
H	-2.160837	5.589303	0.529434
C	-3.407143	-0.520885	-1.353075
C	-3.572236	-1.821257	-1.864913
C	-4.536936	0.291082	-1.165042
C	-4.843761	-2.294130	-2.193005
H	-2.707076	-2.472524	-2.006231
C	-5.809651	-0.191443	-1.486216
H	-4.429617	1.303791	-0.772064
C	-5.966173	-1.481080	-2.000661
H	-4.959283	-3.304498	-2.592799
H	-6.682508	0.448376	-1.334931
H	-6.962226	-1.854923	-2.249932
C	1.364889	-2.350098	1.682622
C	0.724269	-1.299367	2.597638
C	0.103105	-1.847921	3.888782
C	-0.973194	-2.922767	3.701463
C	-2.128494	-2.519478	2.774542
C	-1.813452	-2.581548	1.275066
H	1.438805	-3.301382	2.216600
H	2.360165	-2.036904	1.363672
H	1.482113	-0.535221	2.833223
H	-0.080800	-0.644891	2.128052
H	0.922042	-2.248820	4.509791
H	-0.323392	-1.000402	4.451205
H	-1.369068	-3.171433	4.700154
H	-0.517160	-3.855748	3.323768
H	-2.982183	-3.191532	2.984389
H	-2.484087	-1.514129	3.060869
H	-1.593202	-3.631625	1.007650
H	-2.713740	-2.307542	0.700323
C	0.127222	-2.892247	-1.041480
C	0.950773	-3.458243	-0.023707
H	0.631934	-2.478439	-1.919909
H	-0.831065	-3.378771	-1.246382
H	0.560826	-4.320642	0.520768
H	2.028656	-3.494249	-0.199871
H	-1.321974	2.566859	-2.393616
C	-2.686885	1.167499	1.936331
C	-1.944186	1.333438	3.267294
H	-2.545677	0.143673	1.559549
H	-3.772190	1.256835	2.118510
H	-2.279061	0.581312	3.996926
H	-0.855401	1.223638	3.141632
H	-2.121056	2.322760	3.715090
C	4.129631	-0.137791	1.082220
C	5.031511	1.098009	1.191645
H	4.466049	-0.887020	1.818989
H	3.106138	0.131689	1.375791
H	4.718993	1.884715	0.490902
H	4.995406	1.515915	2.210215
H	6.079466	0.843288	0.967581

^{4}TS9-10C-26
Geometry with 89 atoms:
Total energy: -3202.735218280

Cr	-0.470907	-1.073993	0.934200
P	1.655959	-0.346710	-0.380378
P	-1.404469	0.566241	-0.847106
C	-0.357399	0.188098	-2.328423
C	1.124722	0.428760	-2.009144
H	-0.534873	-0.869686	-2.577083
H	-0.665904	0.784015	-3.200776
H	1.750138	0.003468	-2.806412
H	1.333710	1.507380	-1.979789
C	2.965222	-1.559727	-0.842496
C	2.708080	-2.911796	-0.547292
C	4.172363	-1.200199	-1.497136
C	3.620010	-3.913815	-0.878871
H	1.774630	-3.188414	-0.060639
C	5.071205	-2.230733	-1.821924
C	4.810344	-3.567779	-1.520601
H	3.396993	-4.956453	-0.640945
H	6.001819	-1.970198	-2.334011
H	5.534967	-4.338896	-1.793697
C	2.528534	0.952945	0.588924
C	2.411137	2.329144	0.344319
C	3.288912	0.518906	1.691371
C	3.046174	3.252308	1.181600
H	1.821645	2.703234	-0.492649
C	3.917366	1.443009	2.527733
H	3.407493	-0.549434	1.886269
C	3.797246	2.814462	2.275272
H	2.947332	4.320518	0.973758
H	4.510364	1.090083	3.374977
H	4.292279	3.538261	2.927080
C	-1.191772	2.386975	-0.617991
C	-0.814393	2.976146	0.609141
C	-1.405190	3.205307	-1.747138
C	-0.642112	4.373394	0.649601
C	-1.227991	4.584383	-1.683926
C	-0.837454	5.171217	-0.474551
H	-0.341694	4.837291	1.593141
H	-1.396790	5.199290	-2.570955
H	-0.689394	6.251972	-0.409344
C	-3.149014	0.387235	-1.364534
C	-4.139916	0.919231	-0.518646
C	-3.534980	-0.342711	-2.500953
C	-5.491780	0.721324	-0.804036
H	-3.854205	1.501352	0.361930
C	-4.891087	-0.535454	-2.783342
H	-2.788214	-0.771288	-3.171955
C	-5.870112	-0.009579	-1.935830
H	-6.252710	1.141398	-0.141815
H	-5.181720	-1.101762	-3.671529
H	-6.928424	-0.165266	-2.158568
C	-2.264805	-1.234336	2.186770
C	-3.327420	-2.232389	2.632918
C	-3.983595	-3.039168	1.507183
C	-3.078132	-3.927575	0.638380
C	-2.286917	-3.235747	-0.491536
C	-0.870237	-2.756069	-0.176278
H	-2.179648	-0.387371	2.881853
H	-2.595089	-0.825726	1.212172
H	-2.935406	-2.923944	3.400367
H	-4.126279	-1.666898	3.146278
H	-4.750479	-3.681343	1.972868
H	-4.536890	-2.349051	0.843726
H	-3.733442	-4.676261	0.163471
H	-2.389233	-4.509291	1.278882
H	-2.200067	-3.962203	-1.322445
H	-2.896984	-2.413366	-0.902758
H	-0.316599	-3.549352	0.359150
H	-0.321342	-2.565096	-1.115760
C	0.757195	-1.863447	2.491213
C	-0.502739	-2.264997	2.969848
H	1.272256	-1.033650	2.988916
H	1.405994	-2.595139	2.002992
H	-0.855798	-3.273541	2.742814
H	-0.878830	-1.862720	3.912808
H	-1.725514	2.756942	-2.690709
C	-0.630091	2.220268	1.907734
C	-1.835043	2.345989	2.844856
H	0.276651	2.590192	2.410942
H	-0.428680	1.154437	1.705194
H	-2.746376	1.932042	2.385363
H	-1.657012	1.816275	3.793961
H	-2.034420	3.402623	3.082007
C	4.571589	0.216977	-1.865089
C	5.723737	0.768330	-1.013854
H	3.719255	0.902663	-1.790583
H	4.874982	0.221863	-2.926160
H	5.991973	1.785787	-1.339919
H	5.445484	0.815724	0.049096
H	6.623536	0.139068	-1.099674

^{4}TS9-10C-27
Geometry with 89 atoms:
Total energy: -3202.736561210

Cr	0.269718	-1.064559	1.117348
P	1.705449	0.369120	-0.611710
P	-1.480703	-0.190583	-0.488357
C	-0.669891	0.360175	-2.093700
C	0.816157	-0.014421	-2.206410
H	-1.227392	-0.050621	-2.947802
H	-0.795578	1.451726	-2.125457
H	0.931681	-1.091204	-2.390498
H	1.282298	0.503853	-3.058089
C	3.528290	0.230312	-0.889941
C	4.339881	1.351889	-0.620988
C	4.142391	-0.998652	-1.238350
C	5.729760	1.276290	-0.708507
H	3.884479	2.301890	-0.339475
C	5.543710	-1.047098	-1.324044
C	6.336831	0.069875	-1.064051
H	6.334460	2.161478	-0.497361
H	6.019239	-1.993393	-1.597781
H	7.424845	-0.002751	-1.134377
C	1.416556	2.182939	-0.444678
C	1.159896	2.733927	0.820451
C	1.444836	3.038542	-1.562149
C	0.924491	4.104006	0.969819
H	1.145685	2.094106	1.703304
C	1.202614	4.405210	-1.413886

H	1.665194	2.644851	-2.556756
C	0.938929	4.940734	-0.147829
H	0.721880	4.514284	1.961856
H	1.223414	5.057137	-2.290721
H	0.747186	6.010557	-0.034972
C	-2.489361	1.236999	0.077094
C	-3.481062	1.880936	-0.703822
C	-2.194603	1.717446	1.366905
C	-4.119850	3.004462	-0.150744
C	-2.850569	2.826493	1.897414
C	-3.816162	3.477331	1.126241
H	-4.878497	3.521293	-0.744991
H	-2.606656	3.179774	2.901953
H	-4.336258	4.354629	1.518994
C	-2.662468	-1.512435	-0.948531
C	-3.813424	-1.717705	-0.168180
C	-2.379873	-2.402234	-1.998885
C	-4.669263	-2.787562	-0.443331
H	-4.053734	-1.033564	0.648389
C	-3.241107	-3.467712	-2.272983
H	-1.484148	-2.275203	-2.611555
C	-4.386995	-3.663588	-1.495912
H	-5.564600	-2.932532	0.166030
H	-3.013822	-4.148436	-3.097061
H	-5.059190	-4.497605	-1.711187
C	2.106080	-1.693407	2.172109
C	1.757196	-0.380926	2.876194
C	1.435321	-0.491085	4.369761
C	0.238588	-1.383245	4.715752
C	-1.058417	-1.017731	3.976347
C	-1.171278	-1.577084	2.552925
H	2.357922	-2.451120	2.920277
H	2.947440	-1.568129	1.480734
H	2.581920	0.331246	2.708580
H	0.895356	0.201153	2.419952
H	2.338336	-0.856058	4.887937
H	1.247856	0.526331	4.755580
H	0.078020	-1.317282	5.804392
H	0.482789	-2.442020	4.514090
H	-1.910856	-1.395427	4.572145
H	-1.178424	0.083254	3.979674
H	-1.167987	-2.680662	2.603708
H	-2.150968	-1.300289	2.128479
C	0.161553	-2.935874	0.185459
C	1.137191	-3.267989	1.162214
H	0.470722	-2.889341	-0.864326
H	-0.868866	-3.264640	0.340849
H	0.798168	-3.786781	2.061948
H	2.136099	-3.562178	0.832219
H	-1.438709	1.206349	1.964967
C	-3.913140	1.428659	-2.085891
C	-5.361055	0.921634	-2.135317
H	-3.254127	0.639430	-2.466689
H	-3.805007	2.280609	-2.779558
H	-6.073613	1.694101	-1.806376
H	-5.632652	0.629985	-3.162271
H	-5.493650	0.041949	-1.487921
C	3.365737	-2.255763	-1.564513
C	3.288890	-2.547598	-3.069499
H	2.352646	-2.191006	-1.148341
H	3.843667	-3.111767	-1.059519
H	4.293824	-2.704459	-3.491511
H	2.695717	-3.455484	-3.265503
H	2.831186	-1.711162	-3.620553

^{4}3A-01
Geometry with 65 atoms:
Total energy: -2888.457350300

Cr	-0.143117	-0.176494	1.564525
C	-0.307501	-2.197381	1.521860
C	-1.588455	-2.583997	2.255729
H	-2.441658	-2.516414	1.559399
C	-1.804554	-1.600537	3.414367
C	-1.756149	-0.165467	2.862851
H	-2.698306	0.079057	2.341041
H	-1.611409	0.597619	3.654616
H	-1.003106	-1.748437	4.164119
H	-2.751082	-1.813172	3.945919
H	-1.558590	-3.632574	2.608899
H	-0.156670	-2.679944	0.542511
H	0.597165	-2.397692	2.141111
P	-1.466881	0.228493	-0.433862
C	-1.986824	1.980669	-0.524781
C	-1.883598	2.786051	0.623007
C	-2.259631	4.131921	0.577897
C	-2.745103	4.680114	-0.612037
C	-2.859076	3.882002	-1.756794
C	-2.483810	2.538171	-1.716486
H	-2.590430	1.923122	-2.613393
H	-3.246901	4.308893	-2.684745
H	-3.042150	5.731001	-0.648268
H	-2.179906	4.748681	1.476154
H	-1.532284	2.358437	1.566434
C	-2.957321	-0.791046	-0.689844
C	-2.844627	-2.107382	-1.171446
C	-3.980499	-2.912159	-1.279885
C	-5.232128	-2.417948	-0.898221
C	-5.347138	-1.112894	-0.410339
C	-4.216345	-0.299263	-0.304941
H	-4.318323	0.719969	0.073902
H	-6.322570	-0.722651	-0.110468
H	-6.118210	-3.051990	-0.979656
H	-3.885624	-3.932514	-1.658755
H	-1.873895	-2.520643	-1.454062
C	-0.378513	-0.033484	-1.917635
C	0.979381	0.647189	-1.712782
P	1.822721	0.050990	-0.163170
C	3.181508	1.258177	0.072821
C	2.846573	2.509002	0.623657
C	3.828737	3.483382	0.810391
C	5.156640	3.211785	0.462568
C	5.496592	1.967401	-0.076545
C	4.515146	0.991320	-0.274571
H	4.791087	0.023322	-0.698558
H	6.533171	1.753730	-0.348543
H	5.927437	3.971259	0.614325
H	3.559180	4.453874	1.234121
H	1.810851	2.731416	0.901066
C	2.607174	-1.546989	-0.582260
C	3.221799	-2.263411	0.461613
C	3.826130	-3.496214	0.212632
C	3.808280	-4.037606	-1.077906
C	3.190668	-3.337908	-2.117547
C	2.595079	-2.095772	-1.874406
H	2.128043	-1.562548	-2.704084
H	3.175403	-3.755496	-3.127180
H	4.275628	-5.006103	-1.271537
H	4.307645	-4.039501	1.029134
H	3.235877	-1.853684	1.475736
H	0.857868	1.734334	-1.578438
H	1.637284	0.510897	-2.584879
H	-0.255033	-1.119347	-2.047169
H	-0.887884	0.344369	-2.817663

^{4}3A-02
Geometry with 65 atoms:
Total energy: -2888.454448610

Cr	-0.033146	-0.746458	1.388349
C	0.212823	-2.658202	0.785622
C	0.419605	-2.903865	2.273366
H	0.942938	-3.850150	2.497802
C	-0.918350	-2.739766	3.028813
C	-1.465520	-1.327333	2.744252
H	-2.538714	-1.298134	2.506000
H	-1.282110	-0.633593	3.592987
H	-0.776333	-2.932230	4.105975
H	-1.613685	-3.508830	2.654132
H	1.152391	-2.135205	2.669187
H	-0.692516	-3.129183	0.377641
H	1.093847	-2.861864	0.158608
P	-1.526424	0.051448	-0.364827
C	-2.519419	1.539481	0.013472
C	-2.651167	1.973554	1.342903
C	-3.389717	3.124788	1.635776
C	-3.998952	3.845680	0.605383
C	-3.876118	3.413902	-0.720860
C	-3.142314	2.264781	-1.018380
H	-3.057020	1.932174	-2.056066
H	-4.356580	3.974322	-1.526446
H	-4.574934	4.745540	0.834777
H	-3.490151	3.455918	2.672090
H	-2.190033	1.407289	2.155927
C	-2.703149	-1.218625	-0.952121
C	-4.004802	-1.272378	-0.427069
C	-4.877131	-2.289216	-0.824270
C	-4.458628	-3.259352	-1.740135
C	-3.161631	-3.212134	-2.261359
C	-2.283923	-2.199500	-1.867239
H	-1.272384	-2.181494	-2.278172
H	-2.829547	-3.967205	-2.977893
H	-5.143862	-4.052077	-2.049664
H	-5.890935	-2.319972	-0.417937
H	-4.345807	-0.515887	0.283401
C	-0.491781	0.532391	-1.850705
C	0.895547	-0.125005	-1.866766
P	1.763439	0.104956	-0.235193
C	2.215791	1.884027	-0.208655
C	3.458616	2.352016	-0.667631
C	3.745107	3.719435	-0.642143
C	2.797083	4.630750	-0.164823
C	1.558616	4.172573	0.295305
C	1.271354	2.805384	0.281386
H	0.301656	2.463295	0.654987
H	0.815715	4.878620	0.674267
H	3.026208	5.699009	-0.146295
H	4.715552	4.074903	-0.997213
H	4.207120	1.648357	-1.039477
C	3.333227	-0.822298	-0.347709
C	4.077946	-0.965836	0.838110
C	5.278202	-1.677253	0.838079
C	5.743137	-2.264570	-0.344063
C	5.007120	-2.131460	-1.524457
C	3.807773	-1.411250	-1.531304
H	3.254694	-1.313096	-2.467182
H	5.367777	-2.588173	-2.449259
H	6.679450	-2.827766	-0.343373
H	5.849510	-1.779008	1.763926
H	3.720727	-0.513671	1.768460
H	1.502909	0.295924	-2.683252
H	0.822557	-1.213003	-2.023375
H	-1.045296	0.302838	-2.773855
H	-0.388942	1.626960	-1.797438

^{4}3A-03
Geometry with 65 atoms:
Total energy: -2888.453506190

Cr	-0.089845	-0.524368	1.496096
C	-1.556294	-0.809011	2.900741
C	-1.186636	-2.241358	3.327217
H	-1.103680	-2.353317	4.422120
C	0.143588	-2.627456	2.641822
C	-0.001241	-2.509930	1.131767
H	0.878950	-2.835965	0.556702
H	-0.929172	-2.945511	0.735787
H	0.540844	-3.604317	2.970964
H	0.950777	-1.914705	2.982820
H	-1.957531	-2.953952	2.989839
H	-1.245925	-0.060020	3.662868
H	-2.624997	-0.651812	2.696424
P	-1.509637	0.133415	-0.376804
C	-2.670561	1.523758	-0.143992
C	-3.610225	1.849432	-1.137904
C	-4.461852	2.941012	-0.960333
C	-4.386170	3.709870	0.207319
C	-3.459437	3.385126	1.201796
C	-2.603703	2.293595	1.028187
H	-1.895802	2.031939	1.819006
H	-3.406941	3.976857	2.118791
H	-5.058040	4.560713	0.344136
H	-5.191460	3.191041	-1.734265
H	-3.684396	1.243728	-2.044835
C	-2.519196	-1.270199	-0.974596
C	-3.604738	-1.680078	-0.178668
C	-4.372164	-2.783793	-0.551754
C	-4.060455	-3.495900	-1.715981
C	-2.981445	-3.095788	-2.507707
C	-2.210531	-1.987290	-2.141218
H	-1.374998	-1.694981	-2.779696
H	-2.736297	-3.645411	-3.419773
H	-4.660718	-4.361717	-2.005644
H	-5.217526	-3.090026	0.069081
H	-3.853954	-1.131183	0.732835
C	-0.403490	0.649998	-1.783655

C	0.922670	-0.122314	-1.793106
P	1.811415	0.082458	-0.164553
C	2.340088	1.836560	-0.205555
C	1.784423	2.739437	0.715744
C	2.121691	4.095873	0.671656
C	3.021290	4.557691	-0.292373
C	3.584134	3.663801	-1.212043
C	3.246341	2.310302	-1.171658
H	3.696628	1.616937	-1.886741
H	4.291064	4.024888	-1.962935
H	3.288617	5.616640	-0.326946
H	1.683915	4.789949	1.392975
H	1.083118	2.388444	1.478752
C	3.340033	-0.913324	-0.315663
C	4.515852	-0.487170	0.329091
C	5.664232	-1.281450	0.298216
C	5.653524	-2.510257	-0.369641
C	4.486928	-2.943721	-1.005986
C	3.333772	-2.154351	-0.977761
H	2.435142	-2.516792	-1.481068
H	4.471724	-3.901915	-1.531026
H	6.553803	-3.128933	-0.394236
H	6.572973	-0.936037	0.797250
H	4.541621	0.473843	0.848735
H	1.572980	0.222855	-2.612133
H	0.746319	-1.199394	-1.934774
H	-0.936067	0.549818	-2.742025
H	-0.223931	1.726690	-1.632699

^{4}3A-04
Geometry with 65 atoms:
Total energy: -2888.452585780

Cr	-0.186219	-0.631579	1.447316
C	-0.369853	-2.622580	1.006756
C	-0.421480	-3.087371	2.474218
H	-1.341960	-3.658474	2.679898
C	-0.423495	-1.835534	3.387089
C	-1.519042	-0.873256	2.962536
H	-2.478692	-1.357710	2.734383
H	-1.656195	-0.001931	3.623520
H	0.589075	-1.321307	3.250657
H	-0.384205	-2.078190	4.462832
H	0.433413	-3.734500	2.727077
H	-1.285599	-2.835251	0.434796
H	0.512728	-2.979441	0.453440
P	1.696950	-0.053245	-0.253200
C	2.809500	-1.417837	-0.763088
C	4.059137	-1.572606	-0.137544
C	4.875903	-2.659935	-0.457130
C	4.454494	-3.606393	-1.396591
C	3.210692	-3.461272	-2.017907
C	2.389154	-2.375425	-1.702458
H	1.421248	-2.283673	-2.198780
H	2.875592	-4.195935	-2.754071
H	5.095505	-4.455520	-1.645340
H	5.849107	-2.765344	0.028599
H	4.405328	-0.836529	0.592230
C	2.791495	1.373300	0.085336
C	3.662266	1.880732	-0.896183
C	4.465491	2.986800	-0.614941
C	4.411285	3.593822	0.645989
C	3.552852	3.092958	1.627923
C	2.745046	1.986152	1.348082
H	2.082002	1.595802	2.126345
H	3.512593	3.561190	2.614277
H	5.043444	4.458293	0.863105
H	5.140316	3.376507	-1.380936
H	3.719120	1.406464	-1.879454
C	0.761485	0.439617	-1.802636
C	-0.635399	-0.192059	-1.897608
P	-1.617911	0.140361	-0.354250
C	-3.223408	-0.701942	-0.549950
C	-4.272541	-0.318080	0.305699
C	-5.502804	-0.973267	0.245937
C	-5.696883	-2.022296	-0.660213
C	-4.656377	-2.412245	-1.506902
C	-3.421115	-1.757937	-1.454353
H	-2.624808	-2.080569	-2.127238
H	-4.803412	-3.229609	-2.217010
H	-6.660407	-2.535507	-0.705371
H	-6.313645	-0.664515	0.910030
H	-4.127868	0.499635	1.016608
C	-1.969253	1.933715	-0.412827
C	-2.817822	2.472238	-1.396248
C	-3.034710	3.849818	-1.452066
C	-2.409406	4.698785	-0.530388
C	-1.568438	4.169343	0.452085
C	-1.351087	2.789722	0.512345
H	-0.698178	2.382640	1.289250
H	-1.083774	4.828889	1.175719
H	-2.583965	5.776485	-0.576525
H	-3.697543	4.264298	-2.215475
H	-3.318497	1.813101	-2.110258
H	-0.569697	-1.286019	-2.002717
H	-1.180329	0.194821	-2.773588
H	0.676845	1.536870	-1.757674
H	1.362003	0.194377	-2.691923

^{4}3A-05
Geometry with 65 atoms:
Total energy: -2888.454224090

Cr	-0.173116	-0.517955	1.459123
C	-0.183564	-2.520192	1.207765
C	0.142161	-2.511878	2.692949
H	0.604846	-3.444798	3.060385
C	-1.104238	-2.073065	3.495340
C	-1.579085	-0.713175	2.941880
H	-2.652026	-0.669965	2.704300
H	-1.339402	0.126714	3.627386
H	-0.872841	-2.035450	4.573192
H	-1.880791	-2.843767	3.360534
H	0.969625	-1.758867	2.874459
H	-1.159881	-2.968881	0.979860
H	0.610494	-2.908076	0.552878
P	1.719252	0.070400	-0.274132
C	2.723368	-1.402174	-0.681099
C	2.621629	-2.089706	-1.900371
C	3.359226	-3.259935	-2.111726
C	4.204786	-3.750112	-1.113691
C	4.309698	-3.070550	0.105779
C	3.567190	-1.910091	0.325303
H	3.652869	-1.389804	1.284070
H	4.969598	-3.449131	0.890136
H	4.781372	-4.662497	-1.283572
H	3.272767	-3.787208	-3.064856
H	1.970816	-1.724873	-2.697374
C	2.887818	1.459410	-0.032068
C	4.222671	1.428276	-0.466080
C	5.045088	2.542058	-0.271755
C	4.543344	3.690885	0.347916
C	3.213257	3.727786	0.780404
C	2.390137	2.614795	0.597522
H	1.351282	2.651142	0.941337
H	2.818167	4.622686	1.267337
H	5.190271	4.558873	0.496536
H	6.083425	2.512137	-0.610887
H	4.623288	0.537022	-0.954050
C	0.796799	0.546244	-1.825210
C	-0.563311	-0.153210	-1.939089
P	-1.588447	0.099557	-0.408637
C	-3.140285	-0.816621	-0.703529
C	-3.071837	-2.179063	-1.048107
C	-4.243675	-2.912997	-1.239263
C	-5.490848	-2.299693	-1.077303
C	-5.562768	-0.948643	-0.726918
C	-4.393715	-0.205099	-0.539475
H	-4.463141	0.850916	-0.270062
H	-6.534721	-0.465829	-0.600047
H	-6.407091	-2.876596	-1.224181
H	-4.182300	-3.969261	-1.512239
H	-2.104983	-2.673383	-1.167751
C	-2.007072	1.879695	-0.348110
C	-2.084122	2.683048	-1.498753
C	-2.392640	4.040890	-1.386189
C	-2.632348	4.607122	-0.129542
C	-2.565498	3.812997	1.019363
C	-2.250737	2.455513	0.913226
H	-2.214352	1.837009	1.814289
H	-2.759726	4.250010	2.001748
H	-2.874551	5.669425	-0.046807
H	-2.448617	4.659072	-2.285412
H	-1.907046	2.257555	-2.488749
H	-0.443287	-1.243531	-2.039816
H	-1.119633	0.187977	-2.826451
H	0.667414	1.637773	-1.756610
H	1.422275	0.360074	-2.711997

^{4}3A-06
Geometry with 65 atoms:
Total energy: -2888.453189610

Cr	-0.171403	-0.466691	1.511956
C	-0.266368	-2.486229	1.160712
C	-0.271058	-2.894309	2.644622
H	-1.147205	-3.518133	2.888189
C	-0.346382	-1.603881	3.496193
C	-1.496127	-0.729622	3.029873
H	-2.419527	-1.283978	2.813278
H	-1.694835	0.155020	3.656582
H	0.634994	-1.040178	3.319831
H	-0.283998	-1.784691	4.582859
H	0.629792	-3.469709	2.911473
H	-1.187699	-2.747418	0.618612
H	0.612236	-2.834239	0.597398
P	-1.612326	0.182582	-0.337382
C	-2.078707	1.951641	-0.383894
C	-1.535963	2.836846	0.561357
C	-1.843476	4.199658	0.510783
C	-2.699716	4.683279	-0.482111
C	-3.250770	3.804772	-1.423078
C	-2.943730	2.443973	-1.376443
H	-3.386232	1.760918	-2.106409
H	-3.926372	4.182606	-2.194259
H	-2.944285	5.747558	-0.520777
H	-1.418651	4.882013	1.250773
H	-0.876382	2.465792	1.351506
C	-3.156325	-0.759957	-0.567563
C	-4.163551	-0.598264	0.401720
C	-5.352234	-1.321708	0.305771
C	-5.544402	-2.219543	-0.751034
C	-4.546055	-2.386768	-1.713641
C	-3.353188	-1.660843	-1.626278
H	-2.588971	-1.806162	-2.391738
H	-4.693071	-3.084896	-2.541215
H	-6.474550	-2.788339	-0.822861
H	-6.130925	-1.187493	1.060440
H	-4.017412	0.098018	1.231456
C	-0.591748	-0.056475	-1.872498
C	0.767166	0.645474	-1.730035
P	1.715025	0.066767	-0.230517
C	2.997035	1.352072	0.006242
C	2.791854	2.331278	0.992181
C	3.724482	3.355888	1.175080
C	4.872218	3.403170	0.378273
C	5.086113	2.426776	-0.601497
C	4.154279	1.403794	-0.789865
H	4.331408	0.640398	-1.551586
H	5.985281	2.461462	-1.221481
H	5.605285	4.200457	0.523550
H	3.558358	4.113221	1.945093
H	1.900065	2.295555	1.624893
C	2.617702	-1.439925	-0.750426
C	3.485313	-2.029521	0.188148
C	4.164679	-3.207877	-0.121073
C	3.974957	-3.821464	-1.365209
C	3.107245	-3.248218	-2.297407
C	2.430329	-2.061261	-1.994654
H	1.759766	-1.632047	-2.741366
H	2.955424	-3.723205	-3.269739
H	4.503596	-4.747036	-1.605488
H	4.843232	-3.651441	0.611596
H	3.637868	-1.560146	1.164798
H	0.630880	1.729802	-1.588657
H	1.378605	0.521640	-2.637504
H	-0.461945	-1.141963	-2.008887
H	-1.142980	0.330420	-2.744333

^{4}3A-07
Geometry with 65 atoms:
Total energy: -2888.452007980

Cr	-0.031390	-0.325270	1.525561
C	-1.399945	-0.302277	3.046867
C	-0.945614	-1.590178	3.760445
H	-0.758374	-1.438617	4.837306

C	0.330759	-2.112069	3.060609
C	0.054750	-2.338305	1.582391
H	0.885833	-2.778520	1.010883
H	-0.897269	-2.844698	1.371969
H	0.784203	-2.983888	3.565068
H	1.148223	-1.336248	3.162535
H	-1.717707	-2.372951	3.676968
H	-1.088345	0.609182	3.602575
H	-2.483722	-0.230490	2.874428
P	1.784788	0.043866	-0.280598
C	3.360208	-0.870909	-0.439506
C	3.477756	-2.017534	-1.244464
C	4.674958	-2.739629	-1.269431
C	5.761962	-2.330631	-0.492694
C	5.650467	-1.192602	0.313576
C	4.457797	-0.468035	0.344325
H	4.387042	0.422906	0.973788
H	6.497761	-0.865555	0.921240
H	6.696137	-2.896824	-0.515741
H	4.756103	-3.625918	-1.903432
H	2.645087	-2.359791	-1.861922
C	2.222746	1.821232	-0.286200
C	3.108612	2.390854	-1.216351
C	3.366592	3.762581	-1.183425
C	2.745089	4.575053	-0.226348
C	1.864975	4.016672	0.704990
C	1.609327	2.643060	0.673999
H	0.923162	2.200048	1.407391
H	1.382980	4.647411	1.455583
H	2.952571	5.647669	-0.205015
H	4.058829	4.202175	-1.905613
H	3.605569	1.760150	-1.958054
C	0.879582	-0.204411	-1.888943
C	-0.463770	0.534235	-1.863292
P	-1.510478	0.056069	-0.399711
C	-2.389881	-1.480999	-0.856703
C	-2.173014	-2.156671	-2.067087
C	-2.864329	-3.341888	-2.341936
C	-3.774227	-3.856318	-1.415583
C	-3.992894	-3.186120	-0.205754
C	-3.301010	-2.008604	0.077201
H	-3.469291	-1.494759	1.027054
H	-4.704275	-3.584804	0.521439
H	-4.314735	-4.780327	-1.634660
H	-2.691490	-3.860701	-3.287949
H	-1.471931	-1.770108	-2.808874
C	-2.789304	1.358884	-0.314668
C	-2.729642	2.324896	0.702060
C	-3.671588	3.356765	0.745871
C	-4.678088	3.425670	-0.221511
C	-4.746170	2.460372	-1.233032
C	-3.807489	1.428159	-1.281858
H	-3.873848	0.670431	-2.066883
H	-5.537295	2.509890	-1.985185
H	-5.416852	4.230080	-0.184391
H	-3.623179	4.103129	1.542473
H	-1.957154	2.269318	1.472710
H	-1.028539	0.378685	-2.795708
H	-0.310264	1.620715	-1.763853
H	1.504589	0.140175	-2.728079
H	0.723212	-1.287820	-2.008196

^{43}A-08
Geometry with 65 atoms:
Total energy: -2888.453593570

Cr	0.146913	-0.401160	1.517758
C	0.221207	-2.438133	1.325977
C	0.077715	-2.742756	2.827493
H	-0.875019	-3.248024	3.053614
C	0.164553	-1.404902	3.602561
C	1.365619	-0.597835	3.132323
H	1.558551	0.319283	3.713136
H	2.283931	-1.189368	3.010820
H	0.066991	-1.523088	4.695449
H	-0.786415	-0.820520	3.366172
H	0.890654	-3.398822	3.181200
H	-0.601694	-2.815276	0.700383
H	1.187916	-2.748460	0.904722
P	1.618649	0.130286	-0.361997
C	3.111086	-0.892615	-0.616385
C	3.004158	-2.189515	-1.150283
C	4.140453	-2.993227	-1.270529
C	5.387134	-2.517209	-0.852407
C	5.496387	-1.231823	-0.313368
C	4.365468	-0.420473	-0.193379
H	4.464391	0.583354	0.225796
H	6.468008	-0.854816	0.014878
H	6.273555	-3.149163	-0.945813
H	4.049358	-3.997694	-1.690875
H	2.038588	-2.585154	-1.472751
C	2.161104	1.877028	-0.394988
C	2.652067	2.473516	-1.570194
C	3.045834	3.812651	-1.563458
C	2.958811	4.566515	-0.386828
C	2.482363	3.978247	0.787598
C	2.085503	2.637299	0.784912
H	1.735523	2.177608	1.713897
H	2.423707	4.560745	1.710064
H	3.269518	5.614068	-0.386456
H	3.426781	4.270486	-2.479503
H	2.738587	1.893296	-2.492221
C	0.574689	-0.082042	-1.889418
C	-0.752229	0.675590	-1.754320
P	-1.723205	0.126438	-0.259961
C	-2.624686	-1.389091	-0.747161
C	-2.603817	-1.923323	-2.044687
C	-3.276061	-3.118325	-2.324386
C	-3.977411	-3.784617	-1.316628
C	-4.003794	-3.257277	-0.020047
C	-3.323948	-2.073067	0.265524
H	-3.336863	-1.677397	1.285622
H	-4.549195	-3.775095	0.772597
H	-4.502357	-4.716767	-1.539022
H	-3.252397	-3.526332	-3.337761
H	-2.068354	-1.417684	-2.850353
C	-2.977014	1.444964	-0.055801
C	-2.569993	2.635994	0.572492
C	-3.470006	3.691615	0.731071
C	-4.786687	3.561250	0.275739
C	-5.198629	2.375876	-0.340903
C	-4.299255	1.318895	-0.510144
H	-4.629480	0.397242	-0.994349
H	-6.226704	2.272276	-0.696515
H	-5.493448	4.384629	0.404511
H	-3.145534	4.615289	1.216484
H	-1.542874	2.746064	0.935325
H	-1.364035	0.582295	-2.664854
H	-0.576348	1.754066	-1.609496
H	1.137782	0.252786	-2.774427
H	0.395576	-1.162126	-2.009329

^{43}A-09
Geometry with 65 atoms:
Total energy: -2888.454301790

Cr	0.023287	-0.709565	1.416461
C	1.423242	-1.297525	2.774625
C	0.280755	-2.210290	3.199607
H	0.363356	-2.608538	4.226057
C	0.042454	-3.313370	2.142118
C	-0.193864	-2.648722	0.773723
H	0.550204	-2.912050	0.008751
H	-1.209416	-2.809976	0.378447
H	-0.811762	-3.942001	2.441621
H	0.935212	-3.959931	2.117522
H	-0.677271	-1.603617	3.274868
H	2.305344	-1.842097	2.408689
H	1.712534	-0.547111	3.529020
P	1.534988	0.073976	-0.346346
C	2.647087	-1.249471	-0.942667
C	2.291982	-2.081148	-2.017396
C	3.127138	-3.138429	-2.390979
C	4.315381	-3.376020	-1.694574
C	4.669645	-2.553470	-0.619520
C	3.839379	-1.497196	-0.240057
H	4.124599	-0.859229	0.600055
H	5.598775	-2.734168	-0.073612
H	4.966295	-4.202611	-1.989316
H	2.845765	-3.778126	-3.230937
H	1.363438	-1.920259	-2.569117
C	2.605685	1.514950	-0.003916
C	2.586015	2.124226	1.260938
C	3.372090	3.254433	1.508498
C	4.181343	3.777968	0.496829
C	4.209983	3.170097	-0.764321
C	3.427534	2.042504	-1.016171
H	3.462693	1.567096	-1.999918
H	4.847543	3.575313	-1.553800
H	4.796491	4.659937	0.691148
H	3.355500	3.721687	2.495934
H	1.970060	1.710572	2.063622
C	0.497508	0.601304	-1.809934
C	-0.883980	-0.066837	-1.842837
P	-1.763675	0.130708	-0.209885
C	-3.321807	-0.810562	-0.354250
C	-3.899176	-1.170201	-1.583605
C	-5.095479	-1.893719	-1.611381
C	-5.726442	-2.258392	-0.418392
C	-5.157243	-1.904076	0.809471
C	-3.958313	-1.190058	0.841323
H	-3.513940	-0.925321	1.805510
H	-5.645210	-2.190299	1.744299
H	-6.661526	-2.823094	-0.444650
H	-5.537430	-2.171241	-2.571393
H	-3.426342	-0.889286	-2.526884
C	-2.224341	1.908212	-0.177065
C	-1.281441	2.830120	0.314852
C	-1.567512	4.197538	0.325267
C	-2.803902	4.655832	-0.140355
C	-3.751160	3.743975	-0.617786
C	-3.465754	2.376119	-0.639366
H	-4.213566	1.673151	-1.013648
H	-4.720296	4.099154	-0.976700
H	-3.031705	5.724431	-0.126403
H	-0.824857	4.903936	0.704112
H	-0.313040	2.488008	0.691421
H	-0.808105	-1.151259	-2.023329
H	-1.490187	0.369003	-2.651954
H	0.388721	1.692505	-1.712219
H	1.048687	0.417963	-2.744868

^{43}A-10
Geometry with 65 atoms:
Total energy: -2888.454326710

Cr	0.023038	-0.689577	1.409013
C	1.375863	-1.287637	2.808436
C	0.134242	-2.042709	3.251369
H	0.109928	-2.346401	4.311665
C	-0.182765	-3.204229	2.276086
C	-0.228844	-2.646006	0.842726
H	0.605756	-2.968008	0.203947
H	-1.186706	-2.818669	0.328671
H	-1.136494	-3.677582	2.558741
H	0.609897	-3.963395	2.383377
H	-0.757719	-1.326100	3.218847
H	2.197073	-1.936995	2.473354
H	1.734416	-0.530942	3.524472
P	1.548304	0.049694	-0.358427
C	2.642825	-1.292712	-0.943549
C	2.271695	-2.133999	-2.005000
C	3.092744	-3.205520	-2.369238
C	4.281990	-3.447694	-1.676032
C	4.651321	-2.615837	-0.613217
C	3.835444	-1.545091	-0.243276
H	4.131592	-0.899757	0.587492
H	5.581115	-2.800452	-0.069725
H	4.921957	-4.285294	-1.963618
H	2.799834	-3.852623	-3.199520
H	1.342696	-1.967985	-2.554508
C	2.635381	1.478349	-0.013920
C	2.652075	2.059105	1.264602
C	3.451302	3.178972	1.517146
C	4.237002	3.721201	0.496878
C	4.229588	3.141685	-0.777890
C	3.434288	2.024233	-1.034781
H	3.441160	1.571889	-2.029878
H	4.848939	3.561378	-1.574254
H	4.861746	4.595578	0.694886
H	3.462735	3.623615	2.515079
H	2.055168	1.630136	2.073428
C	0.522082	0.585458	-1.826610
C	-0.869174	-0.062502	-1.857656
P	-1.749070	0.146702	-0.225576
C	-3.309704	-0.789699	-0.373112

C	-3.890078	-1.133498	-1.605656
C	-5.085810	-1.857438	-1.640293
C	-5.713164	-2.238738	-0.450558
C	-5.141189	-1.900053	0.780388
C	-3.942889	-1.185099	0.818936
H	-3.496296	-0.932749	1.785211
H	-5.626521	-2.199384	1.712459
H	-6.647622	-2.804224	-0.481968
H	-5.529859	-2.122530	-2.602856
H	-3.419377	-0.839982	-2.546109
C	-2.197543	1.926834	-0.195256
C	-1.242540	2.842805	0.284771
C	-1.519919	4.211927	0.298103
C	-2.759024	4.677774	-0.152865
C	-3.717456	3.771934	-0.619190
C	-3.441117	2.402215	-0.643530
H	-4.197479	1.703750	-1.008955
H	-4.688426	4.133237	-0.966880
H	-2.980148	5.747734	-0.136120
H	-0.768703	4.913856	0.668225
H	-0.271967	2.494164	0.650210
H	-0.808819	-1.148466	-2.035623
H	-1.469201	0.379440	-2.668153
H	0.428850	1.678651	-1.735199
H	1.071294	0.387823	-2.759849

^{4}3A-11
Geometry with 65 atoms:
Total energy: -2888.453531680

Cr	0.206812	-0.745440	1.388101
C	1.510145	-1.096759	2.911805
C	0.326779	-1.945265	3.340343
H	0.252792	-2.163726	4.419351
C	0.203717	-3.202366	2.444690
C	0.285094	-2.751671	0.974882
H	1.241719	-3.000953	0.493733
H	-0.548579	-3.090139	0.342105
H	-0.740569	-3.727704	2.661393
H	1.027240	-3.889986	2.700529
H	-0.627372	-1.333314	3.184942
H	2.420114	-1.669655	2.685175
H	1.729251	-0.247337	3.579114
P	1.636043	-0.022038	-0.434969
C	3.258343	-0.813548	-0.713425
C	4.439756	-0.165878	-0.313991
C	5.673875	-0.803062	-0.465130
C	5.741512	-2.087434	-1.012858
C	4.568426	-2.737314	-1.409180
C	3.330147	-2.108646	-1.258006
H	2.427056	-2.637673	-1.569585
H	4.615170	-3.741197	-1.838004
H	6.708388	-2.582357	-1.131408
H	6.587020	-0.289162	-0.155121
H	4.402330	0.839128	0.111471
C	1.921290	1.784334	-0.357946
C	1.955333	2.596308	-1.504657
C	2.127121	3.977093	-1.380702
C	2.278252	4.558211	-0.116651
C	2.262138	3.755440	1.027820
C	2.081092	2.374711	0.908819
H	2.072478	1.752095	1.808168
H	2.388540	4.203594	2.016223
H	2.412622	5.638718	-0.024852
H	2.146066	4.602553	-2.276415
H	1.847123	2.158846	-2.499438
C	0.623502	-0.324401	-1.961822
C	-0.746922	0.360177	-1.870537
P	-1.664706	-0.047210	-0.282249
C	-2.935817	-1.285722	-0.729077
C	-3.630751	-1.235541	-1.950836
C	-4.613194	-2.184459	-2.240992
C	-4.917074	-3.187665	-1.313883
C	-4.240133	-3.237596	-0.092098
C	-3.252593	-2.292250	0.199106
H	-2.726377	-2.341897	1.155427
H	-4.476553	-4.017492	0.635567
H	-5.684772	-3.930135	-1.544862
H	-5.146891	-2.138207	-3.193370
H	-3.418793	-0.447434	-2.677695
C	-2.572923	1.503515	0.100839
C	-1.812039	2.656506	0.377263
C	-2.444842	3.852066	0.721286
C	-3.840791	3.907883	0.806412
C	-4.599386	2.763719	0.545097
C	-3.972075	1.563413	0.194738
H	-4.577960	0.678439	-0.010056
H	-5.689538	2.802310	0.610590
H	-4.336376	4.843211	1.077568
H	-1.844443	4.741921	0.925925
H	-0.719909	2.629105	0.317538
H	-1.366396	0.085480	-2.736504
H	-0.636598	1.454165	-1.895058
H	1.173681	0.002788	-2.858375
H	0.508089	-1.417496	-2.038082

^{4}3A-12
Geometry with 65 atoms:
Total energy: -2888.453784500

Cr	0.213369	-0.738379	1.428008
C	1.536238	-1.130160	2.915576
C	0.484762	-2.180686	3.240698
H	0.499552	-2.558573	4.277885
C	0.517020	-3.308541	2.182016
C	0.441786	-2.671456	0.781295
H	1.355929	-2.801911	0.182882
H	-0.435626	-2.987292	0.195736
H	-0.312756	-4.012547	2.354552
H	1.457440	-3.869386	2.311651
H	-0.546706	-1.701814	3.200076
H	2.513846	-1.553741	2.646740
H	1.642834	-0.331527	3.668897
P	1.620895	0.175781	-0.330579
C	3.254465	-0.603694	-0.542388
C	4.198591	-0.419625	0.484818
C	5.455092	-1.019261	0.399190
C	5.777927	-1.817747	-0.704472
C	4.842308	-2.008898	-1.724026
C	3.583029	-1.403935	-1.648424
H	2.870434	-1.563638	-2.459487
H	5.091283	-2.629960	-2.587854
H	6.760494	-2.291393	-0.768151
H	6.183691	-0.867851	1.199219
H	3.948774	0.196173	1.352464
C	1.893651	1.986744	-0.348405
C	0.952248	2.817541	0.284355
C	1.094744	4.206556	0.242288
C	2.185203	4.775744	-0.422538
C	3.130084	3.954235	-1.047224
C	2.987837	2.564988	-1.014150
H	3.733132	1.932108	-1.501447
H	3.984710	4.397693	-1.563944
H	2.302291	5.861729	-0.451217
H	0.354157	4.842588	0.732995
H	0.094685	2.385422	0.806528
C	0.647190	-0.167207	-1.878259
C	-0.766841	0.424075	-1.785011
P	-1.687479	-0.082007	-0.230318
C	-2.823959	-1.422012	-0.752464
C	-2.416874	-2.376499	-1.701077
C	-3.254062	-3.447238	-2.026874
C	-4.500228	-3.579850	-1.407259
C	-4.908395	-2.636277	-0.459103
C	-4.075899	-1.564127	-0.128772
H	-4.411266	-0.830253	0.608246
H	-5.883338	-2.731998	0.025170
H	-5.153468	-4.417186	-1.664006
H	-2.929403	-4.180088	-2.769459
H	-1.446717	-2.293080	-2.195625
C	-2.760710	1.355959	0.133932
C	-2.706335	1.949045	1.405817
C	-3.487635	3.071956	1.697920
C	-4.329380	3.607594	0.719807
C	-4.393693	3.018842	-0.549228
C	-3.615898	1.897848	-0.842836
H	-3.678943	1.440472	-1.833649
H	-5.055605	3.435125	-1.312521
H	-4.940229	4.484972	0.945985
H	-3.439577	3.525249	2.690881
H	-2.054359	1.534266	2.180649
H	-1.360481	0.151752	-2.670780
H	-0.715935	1.523399	-1.754752
H	1.179896	0.245229	-2.749702
H	0.615582	-1.262939	-1.987909

^{4}3A-13
Geometry with 65 atoms:
Total energy: -2888.453317910

Cr	0.071732	-0.830942	1.354196
C	1.004038	-1.474159	3.043625
C	-0.314792	-2.227015	3.131433
H	-0.620777	-2.537906	4.144960
C	-0.355045	-3.371077	2.090271
C	0.000823	-2.777062	0.715181
H	0.969159	-3.111374	0.315497
H	-0.779939	-2.920066	-0.046779
H	-1.352557	-3.838452	2.084096
H	0.370209	-4.142960	2.397403
H	-1.166981	-1.512713	2.868861
H	1.882815	-2.130303	2.978825
H	1.145996	-0.706438	3.822312
P	1.676760	-0.029309	-0.306015
C	3.306571	-0.809299	-0.573156
C	4.173235	-0.317840	-1.565345
C	5.411937	-0.925850	-1.772968
C	5.795257	-2.022363	-0.991043
C	4.940505	-2.507136	0.002375
C	3.698013	-1.902065	0.215603
H	3.036579	-2.274227	0.999366
H	5.241254	-3.358001	0.618340
H	6.766537	-2.495662	-1.154773
H	6.083676	-0.540426	-2.543784
H	3.888119	0.547887	-2.169076
C	1.973394	1.770369	-0.117178
C	1.970811	2.673672	-1.193782
C	2.167791	4.038451	-0.965938
C	2.374263	4.513418	0.333107
C	2.390773	3.619445	1.408681
C	2.189846	2.255087	1.185977
H	2.211726	1.561447	2.032240
H	2.560906	3.984770	2.424297
H	2.525967	5.581483	0.506889
H	2.160090	4.734127	-1.808544
H	1.812738	2.325701	-2.216786
C	0.768238	-0.227955	-1.918471
C	-0.596828	0.474263	-1.904205
P	-1.612208	0.076612	-0.386479
C	-2.836436	-1.204082	-0.835734
C	-2.776845	-1.935650	-2.031945
C	-3.677299	-2.981484	-2.262976
C	-4.641900	-3.306029	-1.306528
C	-4.703191	-2.584937	-0.108216
C	-3.801300	-1.547818	0.131060
H	-3.855306	-0.995636	1.073904
H	-5.453989	-2.834868	0.645270
H	-5.344146	-4.122431	-1.491127
H	-3.621559	-3.543720	-3.198220
H	-2.029090	-1.707917	-2.794072
C	-2.528651	1.627420	-0.054779
C	-1.808531	2.666566	0.564868
C	-2.427823	3.888456	0.833642
C	-3.773259	4.079042	0.499293
C	-4.493504	3.048012	-0.111681
C	-3.876370	1.824975	-0.392753
H	-4.447206	1.027882	-0.873954
H	-5.543418	3.195855	-0.376281
H	-4.261083	5.032475	0.716218
H	-1.859151	4.691012	1.309563
H	-0.754299	2.530072	0.826973
H	-1.168986	0.261547	-2.820016
H	-0.466683	1.565578	-1.869000
H	1.391647	0.138694	-2.749282
H	0.665552	-1.316489	-2.057114

^{4}3A-14
Geometry with 65 atoms:
Total energy: -2888.452014450

Cr	-0.226841	-0.810330	1.364672
C	-0.487961	-2.717835	0.659594
C	-0.374266	-3.407664	2.031991
H	-1.226090	-4.086915	2.203952
C	-0.393682	-2.321722	3.137235
C	-1.503805	-1.317539	2.864364
H	-2.462368	-1.781844	2.594191

H	-1.639839	-0.558547	3.652878
H	0.607221	-1.781446	3.115000
H	-0.376935	-2.744256	4.157022
H	0.543922	-4.011992	2.112787
H	-1.482440	-2.822454	0.201289
H	0.283588	-3.014677	-0.066017
P	1.658502	-0.078269	-0.265517
C	2.872060	-1.330979	-0.841542
C	3.061122	-2.491497	-0.072966
C	4.003723	-3.449662	-0.458476
C	4.765120	-3.256059	-1.613662
C	4.590439	-2.097418	-2.379302
C	3.652735	-1.137382	-1.995121
H	3.545686	-0.230565	-2.595400
H	5.191333	-1.938328	-3.277983
H	5.498827	-4.006318	-1.918119
H	4.140145	-4.350138	0.145143
H	2.471228	-2.654095	0.831951
C	2.672176	1.368964	0.237597
C	2.935991	1.540137	1.607730
C	3.709857	2.615495	2.053084
C	4.224642	3.532657	1.132530
C	3.967924	3.369794	-0.233250
C	3.198017	2.293903	-0.681371
H	3.011959	2.183963	-1.752156
H	4.371389	4.084207	-0.955025
H	4.827331	4.375780	1.478773
H	3.909387	2.737183	3.120529
H	2.540797	0.826209	2.337132
C	0.734865	0.503837	-1.788856
C	-0.661978	-0.124275	-1.909632
P	-1.645674	0.147781	-0.354898
C	-3.271596	-0.637942	-0.595162
C	-3.617552	-1.336148	-1.763110
C	-4.874705	-1.940629	-1.868953
C	-5.790358	-1.849817	-0.817730
C	-5.449255	-1.154703	0.348583
C	-4.194394	-0.556567	0.464113
H	-3.928490	-0.023115	1.379973
H	-6.162169	-1.083386	1.173545
H	-6.771789	-2.322056	-0.905458
H	-5.137843	-2.482588	-2.780512
H	-2.919565	-1.415785	-2.598249
C	-1.935219	1.956116	-0.297701
C	-3.054283	2.548335	-0.907360
C	-3.213676	3.935947	-0.876340
C	-2.261301	4.742191	-0.243421
C	-1.145560	4.159331	0.365201
C	-0.985273	2.771726	0.343157
H	-0.108933	2.331026	0.825983
H	-0.399455	4.783040	0.863242
H	-2.392598	5.826703	-0.220577
H	-4.088057	4.390026	-1.348852
H	-3.805878	1.927165	-1.399907
H	-0.597498	-1.214411	-2.060228
H	-1.200565	0.305808	-2.768901
H	0.647170	1.597459	-1.702508
H	1.319442	0.296004	-2.696754

^{4}3A-15
Geometry with 65 atoms:
Total energy: -2888.453185480

Cr	0.116474	-0.684011	1.438203
C	1.618685	-0.801898	2.799397
C	0.717727	-1.821843	3.489186
H	0.990966	-2.028617	4.539774
C	0.607410	-3.100978	2.630015
C	-0.028961	-2.721955	1.282719
H	0.431192	-3.178011	0.393390
H	-1.116061	-2.912317	1.269015
H	0.018917	-3.871731	3.156716
H	1.620997	-3.512903	2.489502
H	-0.320238	-1.393156	3.585292
H	2.602106	-1.205621	2.520579
H	1.743364	0.147614	3.349191
P	1.497660	0.020554	-0.452280
C	2.857734	-1.050676	-1.034652
C	3.203569	-2.212698	-0.327597
C	4.254975	-3.018388	-0.776392
C	4.965799	-2.668305	-1.927032
C	4.630037	-1.505806	-2.631653
C	3.581969	-0.698213	-2.188727
H	3.336308	0.215342	-2.736652
H	5.189265	-1.226195	-3.527744
H	5.786377	-3.299726	-2.276365
H	4.517532	-3.922710	-0.222328
H	2.657202	-2.487510	0.574130
C	2.241673	1.639844	-0.021029
C	3.608830	1.762053	0.276433
C	4.123214	2.988435	0.707147
C	3.282131	4.095666	0.853271
C	1.917662	3.975770	0.568767
C	1.396299	2.754446	0.137349
H	0.326325	2.680372	-0.072947
H	1.252727	4.835545	0.681637
H	3.689732	5.052175	1.189145
H	5.189511	3.077215	0.928971
H	4.275780	0.904115	0.169018
C	0.411231	0.348031	-1.942700
C	-0.908707	-0.428920	-1.877273
P	-1.795966	-0.148629	-0.261511
C	-3.341114	-1.117914	-0.426983
C	-3.247696	-2.500883	-0.672969
C	-4.404132	-3.278599	-0.760787
C	-5.661983	-2.689691	-0.592066
C	-5.759337	-1.318643	-0.338304
C	-4.606208	-0.532291	-0.255668
H	-4.697071	0.538763	-0.062220
H	-6.739440	-0.853627	-0.206366
H	-6.565680	-3.300419	-0.657334
H	-4.321719	-4.350095	-0.958973
H	-2.272215	-2.977669	-0.798411
C	-2.279785	1.619174	-0.277680
C	-2.610089	2.309829	-1.457121
C	-2.928267	3.669251	-1.410543
C	-2.929886	4.351506	-0.188570
C	-2.617009	3.670745	0.991669
C	-2.290243	2.312572	0.946066
H	-2.042736	1.790725	1.875886
H	-2.623205	4.197516	1.948794
H	-3.178581	5.415065	-0.157086
H	-3.179217	4.198797	-2.332848
H	-2.624286	1.792482	-2.419023
H	-0.731010	-1.515117	-1.937318
H	-1.562201	-0.169447	-2.724111
H	0.223091	1.431383	-1.981925
H	0.968316	0.087425	-2.855046

^{4}3A-16
Geometry with 65 atoms:
Total energy: -2888.452146780

Cr	0.002205	-0.252947	1.541155
C	-1.144177	-0.131077	3.218219
C	0.074320	-0.862240	3.764116
H	1.017087	-0.335170	3.396889
C	0.124330	-2.319012	3.238475
C	0.030546	-2.292752	1.704140
H	0.914196	-2.703167	1.190079
H	-0.884827	-2.737047	1.290091
H	-0.725063	-2.867418	3.678816
H	1.048631	-2.808690	3.584378
H	0.215308	-0.792711	4.856386
H	-1.296417	0.877305	3.636412
H	-2.072345	-0.718279	3.271489
P	1.760448	0.031443	-0.304237
C	3.338734	-0.874119	-0.477069
C	4.436940	-0.460159	0.300158
C	5.639563	-1.166604	0.254055
C	5.760083	-2.297509	-0.561205
C	4.672212	-2.717695	-1.330541
C	3.464556	-2.013469	-1.290277
H	2.630638	-2.363039	-1.902015
H	4.760833	-3.598612	-1.970936
H	6.702348	-2.849474	-0.596684
H	6.487424	-0.831234	0.856372
H	4.358320	0.425635	0.936049
C	2.191191	1.811883	-0.368508
C	1.610228	2.664013	0.586024
C	1.865243	4.038019	0.564200
C	2.711853	4.567465	-0.413689
C	3.300695	3.725183	-1.365535
C	3.043058	2.353105	-1.346336
H	3.514783	1.699767	-2.084961
H	3.967088	4.141855	-2.124681
H	2.918470	5.640294	-0.432809
H	1.408465	4.691657	1.311007
H	0.952101	2.249564	1.360602
C	0.816686	-0.255294	-1.883672
C	-0.529120	0.482140	-1.847639
P	-1.560977	0.020352	-0.366740
C	-2.424945	-1.533002	-0.799787
C	-2.215750	-2.219671	-2.005390
C	-2.897931	-3.414828	-2.258947
C	-3.791058	-3.928536	-1.316040
C	-4.002832	-3.247092	-0.111287
C	-3.320134	-2.059144	0.149946
H	-3.483839	-1.534351	1.095250
H	-4.701555	-3.645294	0.628319
H	-4.323767	-4.860844	-1.518425
H	-2.730736	-3.942205	-3.201267
H	-1.527955	-1.834635	-2.760270
C	-2.864244	1.300438	-0.299541
C	-3.834045	1.381970	-1.314697
C	-4.802733	2.385946	-1.274666
C	-4.813281	3.310925	-0.223657
C	-3.856447	3.228477	0.791532
C	-2.884284	2.224087	0.756989
H	-2.153622	2.150744	1.565668
H	-3.870357	3.942290	1.618725
H	-5.575712	4.093270	-0.193510
H	-5.556404	2.444415	-2.063758
H	-3.840899	0.653300	-2.129478
H	-1.102393	0.315703	-2.772882
H	-0.374929	1.569802	-1.763237
H	1.421531	0.073483	-2.743885
H	0.663080	-1.341785	-1.977024

^{4}3A-17
Geometry with 65 atoms:
Total energy: -2888.452151040

Cr	-0.015072	-0.156423	1.534718
C	1.118401	-0.045018	3.225741
C	-0.191303	-0.555640	3.809009
H	-0.331402	-0.368708	4.887720
C	-0.429820	-2.032580	3.411422
C	-0.237829	-2.162326	1.891068
H	0.682526	-2.687010	1.600212
H	-1.099547	-2.589062	1.354872
H	-1.437409	-2.347919	3.726804
H	0.296236	-2.657621	3.957958
H	-1.052077	0.052126	3.376734
H	1.955138	-0.748135	3.346627
H	1.398848	0.967377	3.558678
P	1.570657	-0.098334	-0.373899
C	2.354911	-1.692590	-0.827415
C	3.743681	-1.809843	-0.999457
C	4.301249	-3.036260	-1.373895
C	3.483091	-4.150215	-1.580582
C	2.099658	-4.040594	-1.403239
C	1.536985	-2.821591	-1.020846
H	0.458257	-2.757253	-0.865215
H	1.455432	-4.909909	-1.555566
H	3.923195	-5.105949	-1.875210
H	5.382722	-3.117663	-1.507382
H	4.394292	-0.946704	-0.846772
C	2.925290	1.127992	-0.269124
C	3.384424	1.836049	-1.394630
C	4.439040	2.743776	-1.269421
C	5.050154	2.947074	-0.027848
C	4.604443	2.239866	1.092808
C	3.544888	1.336840	0.975745
H	3.197940	0.790093	1.854107
H	5.080198	2.392848	2.064466
H	5.875638	3.657099	0.064923
H	4.787531	3.291196	-2.148576
H	2.934348	1.682749	-2.377316
C	0.592805	0.396736	-1.891769
C	-0.819186	-0.200535	-1.934528
P	-1.734154	0.119207	-0.343763
C	-3.319481	-0.768549	-0.477862
C	-3.946331	-1.174025	0.713794
C	-5.175176	-1.836332	0.674546
C	-5.783433	-2.107754	-0.555204

C	-5.161791	-1.715814	-1.745323
C	-3.934929	-1.047618	-1.710711
H	-3.465172	-0.743390	-2.648463
H	-5.635500	-1.929302	-2.706598
H	-6.742695	-2.630055	-0.586713
H	-5.656080	-2.146268	1.605376
H	-3.470787	-0.972294	1.677555
C	-2.102361	1.916337	-0.403735
C	-3.285451	2.458789	-0.928140
C	-3.478645	3.843297	-0.924889
C	-2.497721	4.693962	-0.403165
C	-1.317306	4.161303	0.125561
C	-1.125130	2.778056	0.130382
H	-0.203761	2.363027	0.560620
H	-0.551546	4.820838	0.540820
H	-2.657334	5.774873	-0.401699
H	-4.403647	4.260987	-1.329877
H	-4.060174	1.801459	-1.330131
H	-0.794404	-1.292612	-2.074815
H	-1.375836	0.227092	-2.782983
H	0.534133	1.496514	-1.863937
H	1.156350	0.115883	-2.794267

^{4}3A-18

Geometry with 65 atoms:

Total energy: -2888.446081420

Cr	0.001227	-0.085952	1.523812
C	1.617925	-0.448327	2.687705
C	0.608788	-0.743032	3.805834
H	0.264093	-1.791710	3.755674
C	-0.670546	0.204892	3.864211
C	-1.647581	0.101605	2.685734
H	-2.275728	-0.803477	2.725031
H	-2.277323	0.990113	2.538593
H	-0.322938	1.246182	3.991580
H	-1.189736	-0.058345	4.801094
H	1.099705	-0.632119	4.787350
H	2.263646	-1.297045	2.422990
H	2.232599	0.445915	2.885293
P	-1.550337	-0.067655	-0.431295
C	-3.075843	0.935702	-0.394926
C	-3.043442	2.286221	-0.786223
C	-4.184947	3.082156	-0.661590
C	-5.364832	2.543696	-0.139195
C	-5.399617	1.204495	0.261890
C	-4.262213	0.402856	0.139627
H	-4.303120	-0.641194	0.457709
H	-6.318098	0.778632	0.672985
H	-6.256552	3.167872	-0.043882
H	-4.150813	4.128055	-0.976184
H	-2.129762	2.730271	-1.188620
C	-2.047173	-1.807427	-0.722715
C	-1.445022	-2.819665	0.042422
C	-1.751070	-4.163338	-0.191853
C	-2.668189	-4.502462	-1.190441
C	-3.276006	-3.499278	-1.955342
C	-2.966797	-2.157036	-1.727109
H	-3.450592	-1.379951	-2.324603
H	-3.995571	-3.765028	-2.733453
H	-2.913978	-5.551587	-1.372170
H	-1.278179	-4.943210	0.409707
H	-0.731924	-2.558821	0.832766
C	-0.666777	0.384582	-2.010220
C	0.712549	-0.277952	-2.017272
P	1.579307	0.103561	-0.408852
C	2.020552	1.870402	-0.599340
C	1.387885	2.815253	0.224292
C	1.640353	4.180425	0.059886
C	2.532984	4.606960	-0.927525
C	3.171554	3.670333	-1.749898
C	2.916756	2.307050	-1.590851
H	3.423012	1.580737	-2.232135
H	3.871969	4.005127	-2.518832
H	2.735781	5.672989	-1.056380
H	1.144210	4.908868	0.705537
H	0.691060	2.481314	1.001656
C	3.133532	-0.855502	-0.432792
C	3.123787	-2.196558	-0.857267
C	4.287152	-2.966329	-0.783486
C	5.467265	-2.411687	-0.278293
C	5.479659	-1.082969	0.156615
C	4.319902	-0.307179	0.084779
H	4.343651	0.728722	0.429637
H	6.397876	-0.644553	0.554928
H	6.376201	-3.015485	-0.222380
H	4.270064	-4.004782	-1.123104
H	2.210447	-2.654037	-1.245518
H	1.326729	0.067619	-2.863142
H	0.614943	-1.371996	-2.099780
H	-1.271658	0.077103	-2.877116
H	-0.567544	1.480763	-2.044443

^{4}3A-19

Geometry with 65 atoms:

Total energy: -2888.446653850

Cr	-0.005409	0.086099	1.515797
C	-1.635311	-0.003296	2.715388
C	-0.680290	-0.398157	3.851019
H	-1.124738	-0.123949	4.822913
C	0.754563	0.287000	3.829772
C	1.663309	-0.074843	2.647103
H	2.514305	0.607113	2.513067
H	2.019090	-1.118769	2.676578
H	1.241080	-0.014187	4.773208
H	0.625170	1.383549	3.898567
H	-0.538714	-1.493542	3.876626
H	-2.067953	1.003527	2.848508
H	-2.440540	-0.727754	2.532461
P	1.541945	0.110425	-0.439951
C	2.993648	-0.997695	-0.433478
C	2.795697	-2.372459	-0.659647
C	3.867033	-3.262579	-0.562676
C	5.142250	-2.793873	-0.228676
C	5.341740	-1.431138	0.009142
C	4.274051	-0.534036	-0.088847
H	4.444372	0.527686	0.100607
H	6.334980	-1.059830	0.273115
H	5.979190	-3.492153	-0.151926
H	3.704240	-4.327424	-0.746518
H	1.803490	-2.759491	-0.908060
C	2.138889	1.828447	-0.653606
C	3.001609	2.188581	-1.703955
C	3.383166	3.521366	-1.869290
C	2.904295	4.505079	-0.995301
C	2.045094	4.155643	0.050265
C	1.667136	2.820866	0.220952
H	1.000590	2.544798	1.046122
H	1.672346	4.920098	0.736066
H	3.205107	5.546939	-1.129707
H	4.057592	3.795113	-2.684225
H	3.384492	1.427166	-2.388375
C	0.646420	-0.228163	-2.041324
C	-0.723030	0.454277	-2.005405
P	-1.582353	0.010537	-0.409970
C	-2.017623	-1.752634	-0.658302
C	-2.765458	-2.179543	-1.770148
C	-3.024587	-3.538340	-1.959627
C	-2.537546	-4.482452	-1.047421
C	-1.793882	-4.066788	0.060493
C	-1.538543	-2.706157	0.255103
H	-0.966656	-2.381310	1.130866
H	-1.415908	-4.799843	0.777044
H	-2.741942	-5.544934	-1.200761
H	-3.609578	-3.863349	-2.823432
H	-3.154471	-1.451313	-2.486230
C	-3.135643	0.971867	-0.399547
C	-4.372609	0.372176	-0.110257
C	-5.530110	1.152904	-0.039265
C	-5.464184	2.532985	-0.249655
C	-4.232750	3.137244	-0.525382
C	-3.072137	2.364314	-0.593986
H	-2.116898	2.855685	-0.800309
H	-4.175076	4.216388	-0.687366
H	-6.371578	3.139416	-0.196946
H	-6.488718	0.676597	0.180433
H	-4.439353	-0.704987	0.055367
H	-1.345268	0.163682	-2.865602
H	-0.614542	1.550022	-2.033500
H	1.253687	0.120339	-2.890690
H	0.536961	-1.319670	-2.138854

^{4}3B-01

Geometry with 73 atoms:

Total energy: -3117.380784190

Cr	-0.025075	-0.109129	1.240678
C	1.407743	-0.296165	2.742684
C	0.675854	-0.178720	4.086784
C	-0.686736	-0.870539	3.971452
C	-1.427875	-0.292120	2.761115
H	-1.734924	0.753231	2.959508
H	-2.344922	-0.853248	2.507635
H	-1.267286	-0.778409	4.910263
H	-0.522286	-1.955420	3.824469
H	1.267013	-0.588308	4.928871
H	0.507945	0.888454	4.329207
H	1.781733	-1.328418	2.598280
H	2.286818	0.369933	2.676338
P	1.585766	0.016154	-0.709699
C	3.190853	0.879960	-0.784950
C	3.508445	1.823380	-1.776283
C	4.736713	2.492673	-1.739357
C	5.654700	2.226535	-0.720616
C	5.344100	1.285739	0.268634
C	4.118830	0.619498	0.241966
H	3.883921	-0.113493	1.017304
H	6.059157	1.071446	1.066595
H	6.613517	2.750020	-0.697146
H	4.976345	3.221849	-2.517178
H	2.813380	2.043658	-2.588335
C	1.992480	-1.771763	-0.797949
C	3.073104	-2.257591	-1.550745
C	3.395087	-3.615055	-1.556239
C	2.636170	-4.502354	-0.789943
C	1.556710	-4.046116	-0.028240
C	1.233374	-2.685289	-0.035402
O	0.158231	-2.193632	0.697959
C	-0.869108	-3.120946	1.107089
H	-1.721848	-2.518037	1.429140
H	-0.517654	-3.740940	1.943659
H	-1.162248	-3.751128	0.254596
H	0.989709	-4.755309	0.573408
H	2.884962	-5.566011	-0.773078
H	4.239200	-3.976289	-2.147224
H	3.677056	-1.553950	-2.129221
C	0.697290	0.412231	-2.299272
C	-0.703743	-0.210302	-2.319419
P	-1.594625	0.097112	-0.713688
C	-3.239369	-0.674566	-0.869705
C	-3.567863	-1.577951	-1.894260
C	-4.820690	-2.201246	-1.903619
C	-5.751154	-1.929706	-0.897540
C	-5.428668	-1.030145	0.125740
C	-4.179466	-0.409680	0.144925
H	-3.932015	0.287307	0.949619
H	-6.152744	-0.813409	0.914820
H	-6.728830	-2.417382	-0.909761
H	-5.069408	-2.899151	-2.706860
H	-2.860577	-1.803547	-2.694507
C	-1.890691	1.901434	-0.645595
C	-2.815885	2.533649	-1.491302
C	-3.056594	3.904022	-1.400536
C	-2.370525	4.653361	-0.442162
C	-1.445508	4.050241	0.414250
C	-1.198871	2.675470	0.311533
O	-0.273118	2.039945	1.131355
C	0.563683	2.858347	1.975410
H	1.306785	2.190609	2.416215
H	1.073550	3.621999	1.369845
H	-0.036404	3.326417	2.769190
H	-0.936514	4.661370	1.157134
H	-2.555952	5.725980	-0.348272
H	-3.779764	4.381505	-2.064727
H	-3.362911	1.932306	-2.222315
H	-0.633821	-1.305290	-2.426952
H	-1.289825	0.171481	-3.170171
H	1.286898	0.080875	-3.168346
H	0.621378	1.511193	-2.342697

^{4}3B-02

Geometry with 73 atoms:

Total energy: -3117.380998960

Cr	-0.056634	-0.385245	1.249895
C	1.483670	-0.758569	2.602022

C	0.859937	-1.149453	3.952557
C	-0.484863	-1.846183	3.712828
C	-1.326995	-0.966412	2.781431
H	-1.617008	-0.028844	3.294382
H	-2.264161	-1.453384	2.457151
H	-0.998163	-2.069766	4.668808
H	-0.299359	-2.828638	3.238493
H	1.536499	-1.777082	4.563335
H	0.675455	-0.243519	4.560403
H	2.018103	-1.621763	2.161383
H	2.215827	0.063347	2.693046
P	1.511321	0.075850	-0.711109
C	3.068897	1.026767	-0.707425
C	4.018974	0.714856	0.284725
C	5.208832	1.437827	0.371656
C	5.461876	2.486465	-0.520528
C	4.521666	2.804099	-1.503611
C	3.329326	2.078630	-1.601771
H	2.616118	2.343250	-2.384307
H	4.715535	3.618989	-2.205446
H	6.392874	3.054029	-0.449172
H	5.940950	1.183145	1.141774
H	3.829287	-0.100224	0.986810
C	2.009152	-1.667366	-1.006045
C	3.136661	-2.015420	-1.765424
C	3.500442	-3.351690	-1.938590
C	2.736780	-4.356030	-1.339198
C	1.612480	-4.036131	-0.572435
C	1.252340	-2.695598	-0.409348
O	0.136588	-2.330948	0.339856
C	-0.941934	-3.283952	0.451568
H	-1.821027	-2.727195	0.788259
H	-0.696564	-4.062821	1.187095
H	-1.141218	-3.732997	-0.532478
H	1.037594	-4.832725	-0.101232
H	3.017575	-5.405058	-1.458433
H	4.380260	-3.607098	-2.532849
H	3.740535	-1.223934	-2.216033
C	0.584224	0.578486	-2.244902
C	-0.818169	-0.042150	-2.275129
P	-1.666010	0.159979	-0.627978
C	-3.392799	-0.380697	-0.857281
C	-4.273737	-0.203208	0.226786
C	-5.593877	-0.645365	0.139819
C	-6.046099	-1.283007	-1.021697
C	-5.173475	-1.473325	-2.095996
C	-3.850663	-1.024085	-2.019243
H	-3.189801	-1.180301	-2.873882
H	-5.522242	-1.971095	-3.004193
H	-7.079042	-1.633177	-1.087025
H	-6.272041	-0.496680	0.983577
H	-3.925045	0.284878	1.141152
C	-1.712157	1.977216	-0.403059
C	-2.381111	2.814777	-1.309192
C	-2.346224	4.201593	-1.170324
C	-1.626281	4.761092	-0.111702
C	-0.959294	3.950808	0.810566
C	-1.009760	2.557572	0.674546
O	-0.379555	1.716606	1.584763
C	0.132973	2.297088	2.802549
H	-0.647522	2.898478	3.290345
H	0.408178	1.465488	3.453737
H	1.021412	2.908948	2.587718
H	-0.408736	4.418626	1.624418
H	-1.580665	5.845962	0.008799
H	-2.873459	4.840795	-1.881403
H	-2.941025	2.363607	-2.132955
H	-0.765844	-1.125154	-2.475913
H	-1.420281	0.414704	-3.076253
H	1.154786	0.312511	-3.148299
H	0.500737	1.676076	-2.207860

^{4}3B-03
Geometry with 73 atoms:
Total energy: -3117.378237030

Cr	-0.016626	-0.578175	1.201677
C	1.640246	-0.959746	2.390573
C	1.174467	-2.045134	3.369686
C	-0.196161	-1.652495	3.937056
C	-1.152109	-1.315349	2.778141
H	-1.941308	-0.596129	3.065284
H	-1.671425	-2.223201	2.423224
H	-0.061473	-0.768450	4.588281
H	-0.596953	-2.442278	4.600527
H	1.079060	-3.008400	2.831855
H	1.908232	-2.229246	4.179313
H	2.519290	-1.280916	1.804814
H	1.925385	-0.032504	2.921000
P	1.416456	0.105380	-0.792738
C	2.821395	1.266869	-0.713511
C	3.968578	0.905526	0.019244
C	5.004756	1.822315	0.203210
C	4.908768	3.112097	-0.330526
C	3.768212	3.481508	-1.048144
C	2.727110	2.567923	-1.238086
H	1.843405	2.887712	-1.793128
H	3.684263	4.487661	-1.466216
H	5.721612	3.827834	-0.185771
H	5.892050	1.526485	0.768242
H	4.056079	-0.095842	0.445963
C	2.112743	-1.557425	-1.129700
C	3.274003	-1.775959	-1.885421
C	3.783259	-3.064507	-2.059902
C	3.133462	-4.149740	-1.467570
C	1.971016	-3.959555	-0.713956
C	1.462457	-2.668843	-0.557056
O	0.292792	-2.433343	0.162659
C	-0.706501	-3.473863	0.194245
H	-1.667454	-2.986110	0.390660
H	-0.488180	-4.195455	0.994304
H	-0.744410	-3.980121	-0.781089
H	1.479964	-4.813488	-0.247696
H	3.532647	-5.159901	-1.584310
H	4.688995	-3.218933	-2.649981
H	3.790688	-0.923261	-2.332084
C	0.424074	0.517888	-2.317459
C	-0.957688	-0.147599	-2.262809
P	-1.734272	0.053380	-0.574169
C	-3.502159	-0.352203	-0.777805
C	-3.955561	-1.214541	-1.791130
C	-5.306483	-1.570636	-1.856274
C	-6.212137	-1.073755	-0.915168
C	-5.764352	-0.219532	0.099186
C	-4.417114	0.136328	0.172955
H	-4.075559	0.801767	0.970436
H	-6.468602	0.170896	0.837861
H	-7.267294	-1.351967	-0.970708
H	-5.651455	-2.237034	-2.650725
H	-3.265077	-1.615049	-2.536912
C	-1.655021	1.866468	-0.308176
C	-2.215230	2.773131	-1.222180
C	-2.056692	4.149152	-1.062043
C	-1.320539	4.629936	0.024591
C	-0.761559	3.751297	0.955451
C	-0.938257	2.371080	0.796784
O	-0.416202	1.465636	1.712210
C	-0.086239	1.947432	3.032426
H	-0.905095	2.573802	3.414153
H	0.026106	1.066257	3.668209
H	0.858508	2.509669	3.010579
H	-0.190026	4.152286	1.790928
H	-1.176743	5.704729	0.158135
H	-2.500848	4.841932	-1.779714
H	-2.787685	2.387125	-2.069727
H	-0.876600	-1.231599	-2.445817
H	-1.619184	0.268257	-3.038693
H	0.975435	0.221231	-3.222948
H	0.302745	1.610270	-2.343624

^{4}3B-04
Geometry with 73 atoms:
Total energy: -3117.377709620

Cr	0.018855	0.084062	1.238109
C	-1.408899	0.347616	2.734014
C	-0.629855	0.864990	3.950950
C	0.656813	0.043733	4.083537
C	1.433993	0.137838	2.761986
H	2.167338	-0.680841	2.644871
H	1.994130	1.088748	2.712324
H	0.383007	-1.010136	4.282962
H	1.260355	0.367924	4.953708
H	-0.359540	1.927629	3.796791
H	-1.229528	0.838704	4.881901
H	-2.199415	1.049637	2.411703
H	-1.902147	-0.609780	2.982067
P	-1.599065	-0.004751	-0.712429
C	-3.195445	-0.886000	-0.812507
C	-3.996427	-0.904388	0.345347
C	-5.220746	-1.574028	0.344022
C	-5.655217	-2.241941	-0.806684
C	-4.862422	-2.233154	-1.957254
C	-3.637686	-1.557230	-1.965289
H	-3.041149	-1.559346	-2.879151
H	-5.198082	-2.751953	-2.858589
H	-6.611872	-2.769954	-0.805327
H	-5.836432	-1.577728	1.246784
H	-3.661846	-0.389561	1.248411
C	-2.017898	1.782808	-0.746681
C	-3.128647	2.286419	-1.441103
C	-3.468284	3.638348	-1.372396
C	-2.700322	4.500787	-0.586666
C	-1.592146	4.024988	0.119995
C	-1.249546	2.672821	0.034419
O	-0.141583	2.168683	0.710439
C	0.934112	3.077428	1.028770
H	1.830786	2.467201	1.173780
H	0.707781	3.633452	1.949850
H	1.098396	3.767658	0.189089
H	-1.014196	4.707230	0.742445
H	-2.965648	5.557792	-0.509906
H	-4.335438	4.013877	-1.919559
H	-3.741886	1.601452	-2.032425
C	-0.705985	-0.388033	-2.302034
C	0.714071	0.188625	-2.319256
P	1.608561	-0.102520	-0.712726
C	3.228333	0.722938	-0.882981
C	3.622708	1.421512	-2.036675
C	4.857526	2.078611	-2.071196
C	5.707139	2.041640	-0.962794
C	5.320711	1.344954	0.188316
C	4.087415	0.694167	0.232615
H	3.789413	0.160708	1.137888
H	5.981500	1.312246	1.058008
H	6.671039	2.555282	-0.994379
H	5.156049	2.618494	-2.973228
H	2.980776	1.460000	-2.918507
C	1.960574	-1.895586	-0.611624
C	2.980087	-2.504209	-1.360317
C	3.265247	-3.862159	-1.218445
C	2.531751	-4.622469	-0.304772
C	1.515124	-4.041230	0.457986
C	1.225386	-2.680943	0.303400
O	0.210229	-2.070671	1.033215
C	-0.787066	-2.916629	1.642148
H	-0.378828	-3.412363	2.535054
H	-1.615633	-2.265423	1.931079
H	-1.144054	-3.659238	0.913932
H	0.969321	-4.654178	1.173383
H	2.752328	-5.684196	-0.171524
H	4.060960	-4.321480	-1.808418
H	3.565509	-1.895339	-2.054149
H	0.679761	1.284141	-2.441527
H	1.285229	-0.221754	-3.166645
H	-1.276248	-0.025866	-3.171693
H	-0.672271	-1.488911	-2.360517

^{4}3B-05
Geometry with 73 atoms:
Total energy: -3117.377761620

Cr	-0.020710	-1.134695	0.716099
C	-0.278451	-2.832372	-0.448744
C	-1.378510	-3.672941	0.213233
C	-1.213858	-3.601269	1.735870
C	-1.151086	-2.124965	2.144719
H	-0.773395	-1.972198	3.175678
H	-2.158197	-1.666978	2.110790
H	-0.270177	-4.108666	2.015046
H	-2.018578	-4.160474	2.251743
H	-2.369065	-3.260957	-0.050895
H	-1.377885	-4.720815	-0.146223
H	-0.468749	-2.666856	-1.524734
H	0.700120	-3.346597	-0.376682
P	-1.662851	0.048635	-0.577532

C -3.422905 -0.414716 -0.726111
C -3.796507 -1.436946 -1.617953
C -5.119491 -1.880693 -1.664479
C -6.079789 -1.320168 -0.815972
C -5.711513 -0.314599 0.082211
C -4.389708 0.136200 0.132187
H -4.116535 0.919907 0.841449
H -6.456047 0.123783 0.751176
H -7.114040 -1.670519 -0.852734
H -5.399130 -2.672974 -2.362875
H -3.057620 -1.902690 -2.274458
C -1.611698 1.718049 0.176821
C -2.306122 2.806066 -0.375762
C -2.206101 4.081981 0.177612
C -1.399389 4.276366 1.302105
C -0.703852 3.211553 1.878678
C -0.809951 1.931686 1.320484
O -0.138186 0.845480 1.839685
C 0.695269 1.019218 2.990952
H 0.103313 1.363442 3.852765
H 1.512455 1.725932 2.778084
H 1.118178 0.034094 3.219714
H -0.078336 3.394948 2.750654
H -1.304959 5.271314 1.743432
H -2.752206 4.917861 -0.264205
H -2.938801 2.645090 -1.252782
C -1.046831 0.307449 -2.339696
C 0.457026 -0.005153 -2.538017
P 1.375136 0.114726 -0.934869
C 1.973983 1.825040 -0.736479
C 3.034998 2.085561 0.150338
C 3.417154 3.400845 0.422948
C 2.743723 4.469414 -0.179402
C 1.689061 4.216460 -1.061105
C 1.303135 2.902731 -1.339411
H 0.470983 2.730096 -2.023604
H 1.159255 5.045285 -1.536344
H 3.044514 5.497765 0.034635
H 4.249603 3.592225 1.104775
H 3.572984 1.258489 0.621120
C 2.836228 -0.970101 -0.937579
C 3.774846 -1.002200 -1.978475
C 4.857950 -1.881227 -1.940369
C 5.006515 -2.732041 -0.843604
C 4.090351 -2.713120 0.213321
C 3.005298 -1.831697 0.172048
O 2.069414 -1.762902 1.202359
C 2.283026 -2.572094 2.373662
H 1.471520 -2.334483 3.069252
H 2.239457 -3.642004 2.122118
H 3.251145 -2.324681 2.834680
H 4.235361 -3.393663 1.050182
H 5.847125 -3.428628 -0.800738
H 5.579498 -1.901865 -2.759596
H 3.650995 -0.327055 -2.828962
H 0.898168 0.634640 -3.317010
H 0.588138 -1.051645 -2.850038
H -1.279910 1.349901 -2.602046
H -1.653078 -0.323272 -3.004280

^{4}3B-06
Geometry with 73 atoms:
Total energy: -3117.377062410
Cr -0.051194 -1.099409 0.716101
C -0.214581 -2.796983 -0.474264
C -0.748838 -3.888919 0.464746
C -1.876958 -3.302108 1.323404
C -1.357969 -2.037351 2.018385
H -0.745027 -2.301075 2.906858
H -2.167702 -1.375901 2.375737
H -2.273991 -4.055102 2.031846
H -2.720118 -3.033853 0.660982
H -1.084760 -4.787958 -0.088535
H 0.064147 -4.237944 1.130986
H -0.930743 -2.631368 -1.300004
H 0.749653 -3.074199 -0.936790
P -1.655185 0.078674 -0.593230
C -3.406418 -0.413269 -0.729013
C -4.365949 0.112757 0.152819
C -5.677800 -0.367327 0.129910
C -6.043105 -1.377195 -0.764986
C -5.089861 -1.911910 -1.637622
C -3.776129 -1.439014 -1.618036
H -3.041398 -1.884559 -2.293003
H -5.367637 -2.706551 -2.334066
H -7.069840 -1.750498 -0.780427
H -6.417024 0.050854 0.817443
H -4.093218 0.898239 0.860393
C -1.613966 1.753263 0.145658
C -2.306608 2.836019 -0.418997
C -2.206684 4.116957 0.122939
C -1.401384 4.321308 1.246768
C -0.708170 3.261415 1.835302
C -0.815664 1.976156 1.289980
O -0.150474 0.892780 1.823778
C 0.684489 1.077839 2.971735
H 1.095358 0.092043 3.219825
H 0.096930 1.444599 3.827246
H 1.510472 1.770471 2.746549
H -0.084426 3.452278 2.707019
H -1.306722 5.320432 1.678554
H -2.751300 4.949233 -0.327422
H -2.936218 2.666330 -1.296582
C -1.017828 0.311022 -2.350451
C 0.476914 -0.057780 -2.525136
P 1.390733 0.093423 -0.919757
C 2.014641 1.797641 -0.751804
C 3.079067 2.055033 0.132113
C 3.478834 3.368161 0.389202
C 2.820001 4.438442 -0.226121
C 1.762588 4.188932 -1.105532
C 1.358604 2.877275 -1.367880
H 0.525469 2.708757 -2.051953
H 1.244480 5.019020 -1.591399
H 3.134595 5.465147 -0.024380
H 4.313587 3.556411 1.069106
H 3.604503 1.226067 0.613650
C 2.833790 -1.016042 -0.880461
C 3.785875 -1.086089 -1.906994
C 4.848454 -1.988540 -1.839445
C 4.962277 -2.825581 -0.728139
C 4.032026 -2.769384 0.315252
C 2.968756 -1.864066 0.244816
O 2.018287 -1.762794 1.258795
C 2.228283 -2.511986 2.468637
H 1.416154 -2.239295 3.151666
H 2.179814 -3.593452 2.273482
H 3.196118 -2.244494 2.918987
H 4.146766 -3.442046 1.163487
H 5.785646 -3.540831 -0.663200
H 5.580657 -2.038202 -2.647923
H 3.688829 -0.422891 -2.770351
H 0.941847 0.534108 -3.327906
H 0.573617 -1.121151 -2.790621
H -1.209021 1.360045 -2.620352
H -1.636682 -0.300254 -3.021834

^{4}3B-07
Geometry with 73 atoms:
Total energy: -3117.375064490
Cr -0.120394 -0.997538 0.811000
C -0.439092 -2.796019 -0.190650
C -0.786687 -3.802076 0.913381
C -1.831463 -3.161936 1.836855
C -1.301296 -1.801677 2.303693
H -0.599242 -1.924013 3.157026
H -2.097249 -1.113429 2.639604
H -2.097074 -3.835687 2.674400
H -2.762248 -3.012134 1.259628
H -1.142337 -4.767458 0.502514
H 0.118540 -4.046810 1.502473
H -1.297866 -2.708776 -0.881239
H 0.434402 -3.100083 -0.794402
P -1.693403 0.067191 -0.625913
C -3.463387 -0.350845 -0.743605
C -4.338057 0.132694 0.246484
C -5.681024 -0.246453 0.242993
C -6.164216 -1.114434 -0.742334
C -5.298713 -1.602453 -1.725004
C -3.952061 -1.227072 -1.727986
H -3.293793 -1.625849 -2.501995
H -5.670959 -2.281061 -2.496260
H -7.215806 -1.411026 -0.742911
H -6.353488 0.137199 1.014052
H -3.970451 0.810303 1.021059
C -1.608126 1.826049 -0.131523
C -2.207067 2.850533 -0.880528
C -2.126411 4.180860 -0.468277
C -1.451251 4.488894 0.716940
C -0.849556 3.488015 1.483417
C -0.919343 2.155435 1.057991
O -0.317319 1.126557 1.745457
C 0.321566 1.395885 2.997677
H 1.188761 2.061041 2.861058
H 0.660696 0.428087 3.386782
H -0.390360 1.835481 3.713354
H -0.318439 3.759181 2.394379
H -1.385888 5.525675 1.055456
H -2.594225 4.970242 -1.059984
H -2.753026 2.595125 -1.792781
C -1.006353 -0.053898 -2.357610
C 0.453630 0.430495 -2.468172
P 1.383189 0.162020 -0.874730
C 2.391209 1.662439 -0.577330
C 3.711111 1.560312 -0.101946
C 4.433339 2.710886 0.225646
C 3.851226 3.974277 0.083846
C 2.538624 4.082997 -0.386218
C 1.808900 2.937059 -0.709441
H 0.779686 3.046186 -1.056454
H 2.073725 5.065424 -0.499210
H 4.420049 4.872318 0.336864
H 5.460533 2.617963 0.586927
H 4.184081 0.581809 0.004751
C 2.580388 -1.206743 -1.011262
C 3.333719 -1.493066 -2.155926
C 4.234785 -2.560768 -2.170467
C 4.389141 -3.343014 -1.024595
C 3.650398 -3.075830 0.134072
C 2.746976 -2.011645 0.139601
O 1.970531 -1.701861 1.252210
C 2.327970 -2.270221 2.522630
H 1.710467 -1.764446 3.274199
H 2.114358 -3.349232 2.547635
H 3.391226 -2.083196 2.735603
H 3.779047 -3.709657 1.010340
H 5.089992 -4.181140 -1.023846
H 4.813669 -2.778633 -3.070288
H 3.215154 -0.868530 -3.044932
H 0.489531 1.510907 -2.668055
H 0.967048 -0.063553 -3.306912
H -1.657358 0.485444 -3.063187
H -1.067442 -1.124582 -2.605448

^{4}3B-08
Geometry with 73 atoms:
Total energy: -3117.376187890
Cr 0.103632 -1.239869 0.650593
C 0.143730 -2.861127 -0.647060
C -0.070111 -4.092106 0.244999
C -1.198663 -3.795214 1.240936
C -0.861503 -2.498799 1.986639
H -0.112403 -2.698721 2.781266
H -1.730158 -2.041744 2.494062
H -1.371698 -4.653828 1.918650
H -2.137936 -3.660507 0.673807
H -0.280586 -5.003937 -0.347315
H 0.856905 -4.311628 0.809565
H -0.681408 -2.780191 -1.378480
H 1.086639 -2.915669 -1.220526
P -1.685791 -0.142325 -0.557208
C -3.435999 -0.642880 -0.721087
C -4.007275 -1.376138 0.333040
C -5.351109 -1.752547 0.279725
C -6.134300 -1.404021 -0.825049
C -5.571772 -0.674301 -1.876968
C -4.228240 -0.292854 -1.828851
H -3.811182 0.280053 -2.659441
H -6.181017 -0.399599 -2.741547
H -7.184367 -1.703270 -0.867960
H -5.785245 -2.325878 1.102267
H -3.398511 -1.655092 1.194483
C -1.732365 1.498504 0.271804

C -2.513524 2.555946 -0.217532
C -2.514194 3.802127 0.408363
C -1.724956 3.995881 1.545081
C -0.950847 2.956057 2.064586
C -0.958828 1.706350 1.433950
O -0.217575 0.640810 1.903327
C 0.458468 0.758828 3.159011
H -0.244229 1.049567 3.954772
H 1.284650 1.484016 3.093662
H 0.858748 -0.234554 3.390125
H -0.341258 3.136125 2.948585
H -1.708685 4.968257 2.042693
H -3.127571 4.615171 0.014790
H -3.139425 2.394793 -1.099201
C -1.118321 0.220128 -2.312781
C 0.413586 0.127135 -2.522962
P 1.327940 0.274950 -0.921734
C 1.736778 2.027484 -0.633584
C 2.756899 2.352091 0.279750
C 2.997650 3.684657 0.620366
C 2.222344 4.705834 0.059616
C 1.208390 4.388842 -0.848672
C 0.963682 3.057411 -1.194607
H 0.159551 2.831160 -1.896537
H 0.599143 5.180885 -1.290236
H 2.411878 5.748018 0.327562
H 3.798893 3.927630 1.322786
H 3.373177 1.562726 0.718329
C 2.904391 -0.628290 -1.016691
C 3.808262 -0.495260 -2.080075
C 4.979169 -1.253348 -2.122847
C 5.247999 -2.151801 -1.088534
C 4.366299 -2.297146 -0.012281
C 3.195735 -1.533383 0.029034
O 2.287647 -1.629017 1.082022
C 2.703604 -2.345221 2.258279
H 1.922429 -2.201411 3.011634
H 2.800021 -3.420846 2.050026
H 3.655031 -1.938725 2.633275
H 4.602622 -3.012282 0.773534
H 6.157571 -2.756599 -1.110993
H 5.674883 -1.145501 -2.957437
H 3.586458 0.211424 -2.884101
H 0.761437 0.858244 -3.267787
H 0.678962 -0.875038 -2.890536
H -1.499756 1.214352 -2.589777
H -1.623426 -0.511295 -2.960481

^{4}3B-09
Geometry with 73 atoms:
Total energy: -3117.376301000
Cr 0.112612 -1.231798 0.661457
C -0.003494 -2.866140 -0.601678
C -0.976110 -3.858120 0.049399
C -0.715502 -3.889344 1.561551
C -0.753958 -2.452641 2.098739
H -0.274810 -2.347857 3.092236
H -1.794633 -2.107250 2.234517
H 0.287888 -4.324040 1.734189
H -1.426296 -4.564350 2.076529
H -2.016353 -3.527348 -0.126989
H -0.900010 -4.870347 -0.394166
H -0.265680 -2.648936 -1.652527
H 1.025306 -3.275345 -0.603997
P -1.687464 -0.127465 -0.534299
C -3.445750 -0.605589 -0.704822
C -4.029715 -1.357080 0.329295
C -5.377460 -1.717860 0.264294
C -6.154312 -1.335674 -0.833403
C -5.580306 -0.588659 -1.866668
C -4.232926 -0.223388 -1.806346
H -3.809233 0.362330 -2.624373
H -6.183439 -0.287968 -2.726869
H -7.207468 -1.622302 -0.885718
H -5.819263 -2.305203 1.072720
H -3.429196 -1.666374 1.185748
C -1.715824 1.511549 0.303358
C -2.521791 2.563455 -0.157691
C -2.516126 3.808177 0.471013
C -1.696695 4.006290 1.585172
C -0.895664 2.973332 2.076415
C -0.906896 1.725741 1.441356
O -0.135206 0.670670 1.884694
C 0.707515 0.848361 3.028185
H 1.456957 1.633086 2.842554
H 1.216707 -0.108563 3.190727
H 0.109873 1.090463 3.920316
H -0.263374 3.156909 2.943382
H -1.677658 4.976263 2.087383
H -3.149207 4.615794 0.097971
H -3.172487 2.399171 -1.020415
C -1.130853 0.232930 -2.296411
C 0.396489 0.134474 -2.534267
P 1.331608 0.248399 -0.944529
C 1.765877 1.994318 -0.650355
C 2.815753 2.306209 0.233129
C 3.074893 3.635111 0.575691
C 2.287930 4.664709 0.047842
C 1.244477 4.360401 -0.831027
C 0.981832 3.033244 -1.179625
H 0.155230 2.817410 -1.858358
H 0.625972 5.159095 -1.246948
H 2.491514 5.703702 0.317809
H 3.899265 3.868352 1.254255
H 3.441160 1.510486 0.646226
C 2.892731 -0.679183 -1.050880
C 3.794631 -0.558703 -2.117599
C 4.956861 -1.329754 -2.161879
C 5.220037 -2.227042 -1.124976
C 4.341033 -2.359626 -0.044835
C 3.178583 -1.583304 -0.002448
O 2.273930 -1.663192 1.055060
C 2.643121 -2.458008 2.196889
H 1.846659 -2.331733 2.936608
H 2.715464 -3.521292 1.926095
H 3.597616 -2.101662 2.612710
H 4.574104 -3.073122 0.743551
H 6.123447 -2.840987 -1.148283
H 5.650733 -1.232555 -2.999290
H 3.577722 0.148429 -2.922539
H 0.737518 0.881824 -3.265899
H 0.652142 -0.858938 -2.930459
H -1.511715 1.228977 -2.567710
H -1.649393 -0.495910 -2.936067

^{4}3B-10
Geometry with 73 atoms:
Total energy: -3117.367948980
Cr -0.089972 -1.089857 0.825302
C -1.205845 -2.064927 2.255162
C -2.293003 -2.871677 1.527354
C -1.777265 -3.408016 0.160304
C -0.368182 -2.877524 -0.156047
H -0.147221 -2.876404 -1.238827
H 0.405176 -3.509083 0.320123
H -2.477070 -3.099347 -0.635495
H -1.790605 -4.513835 0.140049
H -2.677647 -3.700491 2.151464
H -3.162154 -2.215876 1.351660
H -0.491588 -2.740451 2.767757
H -1.632281 -1.394012 3.025025
P 1.342914 0.049184 -0.917719
C 2.292801 1.579737 -0.589573
C 2.397495 2.668779 -1.466677
C 3.097804 3.817086 -1.080928
C 3.702550 3.887200 0.176249
C 3.610384 2.799771 1.053159
C 2.906806 1.656081 0.675662
H 2.829609 0.812549 1.366561
H 4.087191 2.845402 2.035588
H 4.249427 4.785678 0.472224
H 3.172578 4.659332 -1.773125
H 1.941359 2.640258 -2.458360
C 2.603394 -1.269954 -1.016938
C 3.361530 -1.566137 -2.154859
C 4.299891 -2.601569 -2.138193
C 4.485056 -3.340160 -0.968742
C 3.742948 -3.059695 0.184991
C 2.804926 -2.026657 0.160064
O 2.028012 -1.694464 1.271324
C 2.337571 -2.301251 2.535601
H 2.112553 -3.378397 2.522023
H 1.699824 -1.809646 3.279865
H 3.395533 -2.134189 2.788138
H 3.901093 -3.658985 1.080402
H 5.214048 -4.153540 -0.944072
H 4.882911 -2.828564 -3.033110
H 3.217377 -0.976958 -3.064248
C 0.400257 0.244335 -2.507234
C -1.079036 -0.167226 -2.330763
P -1.688877 0.031172 -0.577969
C -3.498761 -0.182200 -0.642191
C -4.119407 -0.966822 -1.628632
C -5.501112 -1.176426 -1.589159
C -6.270554 -0.611219 -0.568731
C -5.656273 0.168917 0.417379
C -4.277511 0.381204 0.384824
H -3.805386 0.990630 1.159705
H -6.253794 0.613627 1.216801
H -7.349986 -0.778314 -0.540961
H -5.976422 -1.785548 -2.361749
H -3.538138 -1.422056 -2.432611
C -1.403498 1.784631 -0.124194
C -1.863466 2.851986 -0.910470
C -1.603804 4.173513 -0.547438
C -0.883953 4.433712 0.622210
C -0.422983 3.390506 1.428928
C -0.678024 2.066485 1.055035
O -0.222548 0.989847 1.788489
C 0.269248 1.199021 3.116888
H -0.480462 1.722692 3.729979
H 0.444277 0.202922 3.542183
H 1.212680 1.765485 3.103792
H 0.146046 3.619805 2.328699
H -0.672176 5.464359 0.916402
H -1.963678 4.995601 -1.169445
H -2.436628 2.638864 -1.816886
H -1.210937 -1.236917 -2.553957
H -1.725156 0.395285 -3.022268
H 0.871406 -0.326838 -3.320710
H 0.453412 1.306116 -2.781300

^{4}5A-01
Geometry with 71 atoms:
Total energy: -2967.044793450
Cr -0.065208 -0.811324 1.083741
C 0.073744 -2.583737 0.059921
C 1.074234 -3.588694 0.630366
H 1.128195 -4.446253 -0.067174
H 2.094188 -3.160255 0.633227
C 0.725898 -4.129766 2.026633
H 1.232970 -5.096524 2.179719
C 1.116135 -3.219711 3.200165
C 0.616479 -1.770542 3.123051
C -0.841177 -1.538343 2.808725
H -1.319143 -0.762597 3.428221
H -1.464209 -2.440183 2.763620
H 0.956563 -1.202124 4.004664
H 1.293560 -1.268691 2.316647
H 0.733697 -3.654201 4.139197
H 2.216126 -3.202325 3.292249
H -0.354745 -4.353052 2.062918
H 0.339058 -2.319777 -0.978511
H -0.945671 -3.007063 0.049922
P -1.759303 0.093501 -0.451672
C -3.348990 -0.738942 -0.783437
C -4.211271 -0.281173 -1.794945
C -5.425934 -0.929585 -2.021901
C -5.789377 -2.032607 -1.239557
C -4.938696 -2.485312 -0.227485
C -3.719654 -1.840766 0.003658
H -3.056884 -2.190540 0.798212
H -5.223549 -3.343147 0.386369
H -6.741657 -2.537704 -1.419176
H -6.094227 -0.571517 -2.808724
H -3.941424 0.587522 -2.401173
C -2.138330 1.825370 0.025347
C -2.268010 2.870787 -0.904464
C -2.518656 4.173956 -0.466566
C -2.648172 4.445697 0.899298
C -2.531957 3.409644 1.831340
C -2.276116 2.106368 1.397635
H -2.191541 1.299443 2.132152

H	-2.640585	3.615955	2.898872
H	-2.842264	5.466621	1.236883
H	-2.612996	4.981316	-1.196825
H	-2.169657	2.679973	-1.975284
C	-0.889167	0.207595	-2.091494
C	0.443518	0.964186	-1.988260
P	1.509701	0.431903	-0.541905
C	2.800716	-0.690754	-1.185369
C	2.665606	-1.365246	-2.408880
C	3.615327	-2.316089	-2.797398
C	4.705653	-2.600383	-1.971881
C	4.844712	-1.934235	-0.748587
C	3.894410	-0.992636	-0.351838
H	4.007962	-0.484964	0.610141
H	5.695038	-2.153082	-0.098158
H	5.446646	-3.342129	-2.279053
H	3.499327	-2.835527	-3.751640
H	1.817969	-1.164926	-3.067382
C	2.337949	1.981818	-0.028734
C	1.643358	2.811427	0.870664
C	2.186664	4.037015	1.261529
C	3.432052	4.438371	0.766775
C	4.128250	3.615807	-0.125075
C	3.584753	2.392575	-0.527660
H	4.133999	1.759493	-1.228071
H	5.099867	3.929566	-0.514552
H	3.861452	5.394103	1.077085
H	1.637358	4.677087	1.956173
H	0.665315	2.509312	1.257772
H	0.259531	2.034435	-1.812323
H	1.015235	0.896229	-2.926703
H	-0.746263	-0.835954	-2.413930
H	-1.543896	0.679633	-2.840948

^{4}5A-02
Geometry with 71 atoms:
Total energy: -2967.043244440

Cr	-0.288916	-0.812608	1.071587
C	-0.678645	-2.572771	0.092682
C	-0.403640	-3.848792	0.891172
H	-0.573942	-4.712017	0.219756
H	0.663776	-3.919138	1.177712
C	-1.277863	-4.036558	2.142527
H	-1.325896	-5.108359	2.395034
C	-0.792743	-3.293178	3.395758
C	-0.542796	-1.788290	3.227709
C	-1.629532	-0.973309	2.572954
H	-1.823511	0.001187	3.049662
H	-2.563916	-1.505779	2.358630
H	-0.193965	-1.349829	4.177594
H	0.443216	-1.711947	2.614998
H	-1.536001	-3.418450	4.201209
H	0.138050	-3.763918	3.757574
H	-2.313593	-3.741183	1.901143
H	-0.064993	-2.537585	-0.825917
H	-1.741723	-2.531715	-0.202165
P	-1.576228	0.482761	-0.546613
C	-3.246175	-0.106140	-0.970027
C	-4.209353	-0.103107	0.056565
C	-5.499943	-0.569678	-0.191603
C	-5.838807	-1.054342	-1.460700
C	-4.884004	-1.067280	-2.480459
C	-3.589229	-0.594142	-2.240792
H	-2.859359	-0.611387	-3.052298
H	-5.145129	-1.445775	-3.471602
H	-6.849175	-1.423473	-1.652522
H	-6.243876	-0.559064	0.608701
H	-3.947447	0.267724	1.050891
C	-1.729630	2.263220	-0.143103
C	-2.681430	3.085263	-0.770122
C	-2.726150	4.450283	-0.477094
C	-1.823588	5.005763	0.437100
C	-0.876756	4.193215	1.067835
C	-0.834216	2.825994	0.783500
H	-0.091843	2.199094	1.286324
H	-0.172458	4.620860	1.785270
H	-1.862303	6.074509	0.661555
H	-3.470380	5.084426	-0.964959
H	-3.393033	2.659157	-1.481675
C	-0.547724	0.447525	-2.094699
C	0.861175	0.986323	-1.804493
P	1.708192	0.075747	-0.400605
C	2.824372	-1.136144	-1.214221
C	3.689381	-0.758517	-2.256533
C	4.539916	-1.699808	-2.838225
C	4.541588	-3.023661	-2.381507
C	3.695088	-3.402474	-1.336912
C	2.839701	-2.461950	-0.754316
H	2.181829	-2.764193	0.061696
H	3.696643	-4.432789	-0.973112
H	5.208355	-3.758275	-2.839670
H	5.208638	-1.399363	-3.648513
H	3.712857	0.275772	-2.609548
C	2.834767	1.318270	0.346217
C	3.224801	1.123936	1.682797
C	4.103798	2.016496	2.301834
C	4.597304	3.115933	1.592927
C	4.213397	3.317611	0.263185
C	3.338468	2.424247	-0.360349
H	3.057297	2.598116	-1.401369
H	4.599608	4.174238	-0.294618
H	5.282619	3.816309	2.076375
H	4.402240	1.853537	3.340284
H	2.848298	0.263523	2.244606
H	0.798942	2.043498	-1.505734
H	1.479194	0.938849	-2.712897
H	-0.512059	-0.600048	-2.436087
H	-1.031639	1.044811	-2.883805

^{4}5A-03
Geometry with 71 atoms:
Total energy: -2967.044626050

Cr	-0.074973	-0.133272	1.312919
C	-0.005691	-2.172871	1.279251
C	0.826887	-2.844435	2.369993
H	0.842509	-3.932096	2.164669
H	1.885562	-2.529505	2.303908
C	0.312255	-2.634757	3.802478
H	0.705243	-3.433827	4.452193
C	0.697197	-1.292849	4.441172
C	0.351532	-0.038629	3.627343
C	-1.043520	0.084420	3.071797
H	-1.482029	1.089023	3.176077
H	-1.754276	-0.695962	3.370532
H	0.677311	0.867056	4.165755
H	1.131243	-0.018900	2.759120
H	0.198493	-1.200241	5.420696
H	1.782373	-1.287751	4.644521
H	-0.784645	-2.758442	3.809061
H	0.383949	-2.423897	0.276295
H	-1.060120	-2.491994	1.338870
P	-1.712149	0.163588	-0.541294
C	-3.069457	-1.015500	-0.886477
C	-2.744624	-2.375420	-1.045816
C	-3.745552	-3.307021	-1.327730
C	-5.077274	-2.894085	-1.443215
C	-5.404241	-1.544918	-1.281659
C	-4.406857	-0.604957	-1.005732
H	-4.676352	0.446176	-0.888055
H	-6.442459	-1.216777	-1.373768
H	-5.860257	-3.624964	-1.659065
H	-3.484169	-4.360614	-1.452454
H	-1.710841	-2.714132	-0.949436
C	-2.478676	1.820636	-0.378274
C	-2.416141	2.802899	-1.380988
C	-3.012331	4.051830	-1.179863
C	-3.681983	4.328881	0.015230
C	-3.755157	3.353500	1.015856
C	-3.150966	2.109518	0.825695
H	-3.211359	1.353088	1.612002
H	-4.282068	3.563106	1.949900
H	-4.148566	5.305223	0.167232
H	-2.956711	4.809259	-1.965523
H	-1.911198	2.606660	-2.328474
C	-0.731140	0.182974	-2.123627
C	0.591205	0.949065	-1.997358
P	1.639010	0.335838	-0.584586
C	2.496863	-1.164106	-1.186364
C	3.324797	-1.841099	-0.271299
C	3.984407	-3.011726	-0.645932
C	3.813677	-3.530672	-1.934776
C	2.987757	-2.869190	-2.846727
C	2.332509	-1.688874	-2.478427
H	1.699426	-1.188310	-3.213508
H	2.852925	-3.268951	-3.854718
H	4.324782	-4.451374	-2.226295
H	4.629452	-3.524114	0.071840
H	3.457915	-1.447700	0.740303
C	2.928574	1.622865	-0.401626
C	4.172416	1.549018	-1.049415
C	5.109093	2.572445	-0.879974
C	4.811661	3.674140	-0.071232
C	3.573409	3.753843	0.574911
C	2.637816	2.729178	0.415910
H	1.675207	2.794351	0.933656
H	3.339123	4.611128	1.210672
H	5.548084	4.470849	0.059375
H	6.076894	2.508064	-1.383256
H	4.413860	0.690055	-1.679838
H	0.411819	2.013025	-1.776253
H	1.164374	0.919649	-2.937189
H	-0.554188	-0.877927	-2.361704
H	-1.355544	0.583303	-2.937772

^{4}5A-04
Geometry with 71 atoms:
Total energy: -2967.044961430

Cr	-0.166692	-0.697516	1.138523
C	-0.440587	-2.540447	0.285326
C	0.004241	-3.741189	1.122425
H	-0.140767	-4.651550	0.509779
H	1.092169	-3.705841	1.322156
C	-0.749810	-3.934300	2.448311
H	-0.669641	-4.988162	2.761198
C	-0.248279	-3.071505	3.615427
C	-0.174842	-1.561784	3.349225
C	-1.387621	-0.904023	2.738941
H	-1.665967	0.057622	3.198565
H	-2.267000	-1.547149	2.611122
H	0.192708	-1.031817	4.243609
H	0.752714	-1.420197	2.658963
H	-0.908013	-3.222748	4.486416
H	0.753051	-3.422407	3.920746
H	-1.825371	-3.755863	2.276859
H	0.115363	-2.500035	-0.669375
H	-1.517925	-2.612258	0.057448
P	-1.602304	0.357876	-0.551943
C	-3.171025	-0.484064	-0.950583
C	-4.159587	-0.515044	0.050412
C	-5.363993	-1.181828	-0.174009
C	-5.589479	-1.832096	-1.393230
C	-4.608024	-1.810258	-2.387022
C	-3.399500	-1.139298	-2.170612
H	-2.646670	-1.135665	-2.960723
H	-4.780650	-2.316990	-3.339656
H	-6.531891	-2.357139	-1.566977
H	-6.128892	-1.197557	0.606176
H	-3.985895	-0.016154	1.007897
C	-2.026654	2.118311	-0.273075
C	-2.673785	2.869885	-1.269832
C	-2.960814	4.218640	-1.054679
C	-2.608943	4.828957	0.155595
C	-1.975439	4.086429	1.155190
C	-1.686786	2.734187	0.942935
H	-1.204072	2.158324	1.736719
H	-1.708923	4.556864	2.104644
H	-2.836208	5.885056	0.320106
H	-3.464523	4.796776	-1.833124
H	-2.963551	2.400952	-2.213859
C	-0.575576	0.369635	-2.099793
C	0.781582	1.034053	-1.833389
P	1.718059	0.212773	-0.431524
C	2.863735	-0.976400	-1.220623
C	3.069785	-2.221489	-0.604813
C	3.961429	-3.145885	-1.156601
C	4.653100	-2.833628	-2.329862
C	4.458715	-1.592182	-2.946848
C	3.571777	-0.665529	-2.395529
H	3.446200	0.306121	-2.879064
H	5.005014	-1.342642	-3.859736
H	5.347674	-3.556644	-2.764529
H	4.111875	-4.112075	-0.669069
H	2.531780	-2.473314	0.310724

C 2.774244 1.555162 0.247395
C 4.161509 1.404648 0.406332
C 4.914244 2.420621 1.004115
C 4.294552 3.591223 1.449736
C 2.911800 3.744798 1.300441
C 2.154055 2.731968 0.709669
H 1.074546 2.871636 0.604585
H 2.418938 4.657157 1.645471
H 4.887231 4.383619 1.913071
H 5.993826 2.294672 1.117567
H 4.661779 0.497973 0.060230
H 0.643595 2.089083 -1.551538
H 1.397735 1.031601 -2.744463
H -0.447405 -0.678883 -2.413814
H -1.112699 0.892875 -2.906495

^{4}5A-05
Geometry with 71 atoms:
Total energy: -2967.044132920
Cr 0.102970 -0.409667 1.246288
C 1.562693 -0.417940 2.682304
C 1.256433 -1.178168 3.979030
H 2.086714 -1.027121 4.694414
H 0.366920 -0.750088 4.481286
C 1.050731 -2.691912 3.790819
H 1.265039 -3.214530 4.737459
C -0.362797 -3.103416 3.351783
C -0.922852 -2.383586 2.117686
C -0.065549 -2.372174 0.874078
H -0.590437 -2.626367 -0.056305
H 0.889604 -2.906320 0.948808
H -1.951088 -2.719288 1.905117
H -1.140366 -1.303646 2.459490
H -0.377071 -4.186283 3.140673
H -1.060847 -2.942522 4.191797
H 1.797609 -3.067257 3.068972
H 1.648844 0.675027 2.876909
H 2.541190 -0.730523 2.277493
P 1.544876 0.330815 -0.616111
C 2.836197 1.582747 -0.285544
C 2.489228 2.674962 0.529943
C 3.422711 3.676508 0.800014
C 4.714210 3.588388 0.268499
C 5.066186 2.500885 -0.536151
C 4.132481 1.498590 -0.816978
H 4.417838 0.653164 -1.446632
H 6.074879 2.429916 -0.950205
H 5.448089 4.368210 0.485744
H 3.144880 4.523257 1.432244
H 1.483450 2.748645 0.954755
C 2.361526 -1.087880 -1.431298
C 2.201974 -1.381672 -2.795289
C 2.842181 -2.493090 -3.353983
C 3.648346 -3.313678 -2.561379
C 3.812757 -3.025156 -1.201726
C 3.168257 -1.924353 -0.636692
H 3.297914 -1.712207 0.426617
H 4.442628 -3.662883 -0.576931
H 4.149587 -4.178918 -3.001880
H 2.711917 -2.712895 -4.416379
H 1.585855 -0.750860 -3.438192
C 0.442416 1.130957 -1.883761
C -0.889053 0.389336 -2.045819
P -1.782370 0.286955 -0.409605
C -2.400080 1.992477 -0.153755
C -3.164877 2.660435 -1.127009
C -3.581528 3.974873 -0.911209
C -3.241540 4.635103 0.276261
C -2.488128 3.977811 1.252353
C -2.070301 2.660421 1.037772
H -1.488073 2.149035 1.811491
H -2.227416 4.488430 2.182408
H -3.569262 5.664467 0.440614
H -4.176189 4.487372 -1.671313
H -3.444954 2.148966 -2.051822
C -3.246896 -0.763220 -0.730918
C -3.093235 -1.989373 -1.405592
C -4.186264 -2.842141 -1.576676
C -5.441275 -2.487520 -1.071844
C -5.599162 -1.275023 -0.394014
C -4.510127 -0.416540 -0.220326
H -4.650798 0.529395 0.307389
H -6.577533 -0.991315 0.001497
H -6.295065 -3.155671 -1.207327
H -4.055137 -3.787718 -2.108457
H -2.122447 -2.288446 -1.807329
H -0.723800 -0.641390 -2.395836
H -1.530960 0.889802 -2.787495
H 0.275405 2.156727 -1.516131
H 0.976233 1.229404 -2.841592

^{4}5A-06
Geometry with 71 atoms:
Total energy: -2967.045863700
Cr -0.151750 -0.663254 1.154655
C -0.346677 -2.476395 0.224191
C 0.304146 -3.646623 0.962810
H 0.223143 -4.540473 0.315143
H 1.392254 -3.479762 1.079111
C -0.325184 -3.985478 2.324816
H -0.117013 -5.039751 2.570162
C 0.167929 -3.136578 3.505973
C 0.093994 -1.615735 3.313592
C -1.212845 -1.032693 2.831748
H -1.511155 -0.100394 3.338632
H -2.051607 -1.737413 2.771608
H 0.489483 -1.097815 4.203346
H 0.951193 -1.375076 2.564146
H -0.418715 -3.389756 4.405241
H 1.214160 -3.407197 3.731593
H -1.423249 -3.912336 2.236657
H 0.094974 -2.355194 -0.780923
H -1.431605 -2.643335 0.107800
P -1.673367 0.387553 -0.466005
C -3.252987 -0.455011 -0.806950
C -4.073311 -0.760034 0.294876
C -5.291556 -1.412738 0.103740
C -5.696641 -1.778189 -1.185223
C -4.882803 -1.483794 -2.282257
C -3.664187 -0.822460 -2.098786
H -3.047221 -0.599048 -2.971081
H -5.195979 -1.768130 -3.289772
H -6.647633 -2.295446 -1.333779
H -5.923801 -1.644064 0.964285
H -3.754986 -0.487715 1.304553
C -2.062128 2.151138 -0.153256
C -3.261057 2.740966 -0.586406
C -3.495242 4.099144 -0.355025
C -2.539178 4.878271 0.304875
C -1.344170 4.296886 0.740355
C -1.108588 2.938162 0.518387
H -0.170219 2.499048 0.867226
H -0.594024 4.899625 1.257927
H -2.727681 5.939690 0.483406
H -4.431228 4.551027 -0.692354
H -4.015249 2.141070 -1.100820
C -0.714708 0.402598 -2.061635
C 0.684015 1.007249 -1.867551
P 1.649510 0.244643 -0.454538
C 2.733515 -1.028608 -1.202057
C 2.381432 -1.702649 -2.383234
C 3.185066 -2.739351 -2.868235
C 4.341914 -3.114259 -2.180080
C 4.696331 -2.448646 -1.001405
C 3.896330 -1.415161 -0.510845
H 4.186867 -0.899230 0.408316
H 5.602179 -2.734321 -0.461044
H 4.968485 -3.923900 -2.561651
H 2.903952 -3.254771 -3.789834
H 1.480773 -1.429120 -2.936879
C 2.771930 1.586648 0.083066
C 2.660995 2.090906 1.389137
C 3.473183 3.149157 1.809948
C 4.402924 3.706098 0.927981
C 4.524644 3.203169 -0.373423
C 3.715271 2.147569 -0.796108
H 3.822604 1.752353 -1.809541
H 5.256148 3.634973 -1.060753
H 5.039132 4.531999 1.255356
H 3.381901 3.534279 2.828379
H 1.941624 1.655630 2.089496
H 0.600396 2.076049 -1.616232
H 1.268883 0.944555 -2.798053
H -0.659741 -0.644714 -2.399007
H -1.271325 0.972474 -2.822346

^{4}5A-07
Geometry with 71 atoms:
Total energy: -2967.045032880
Cr 0.195131 -0.643210 1.161800
C 1.735321 -0.766261 2.506563
C 1.645589 -1.873940 3.562937
H 2.486096 -1.764897 4.274207
H 0.733443 -1.755735 4.180038
C 1.685936 -3.299191 2.983692
H 2.045612 -4.000662 3.754311
C 0.337186 -3.831711 2.475921
C -0.414690 -2.935826 1.482097
C 0.350346 -2.441358 0.276144
H -0.189392 -2.539130 -0.676282
H 1.384287 -2.799405 0.194242
H -1.375302 -3.393135 1.194801
H -0.803655 -2.042792 2.099362
H 0.493989 -4.809407 1.989023
H -0.323695 -4.019252 3.340248
H 2.437861 -3.333936 2.175668
H 1.671098 0.238180 2.983304
H 2.709750 -0.810546 1.989505
P 1.500184 0.504027 -0.542576
C 1.869583 2.276588 -0.273133
C 2.526063 3.033795 -1.260506
C 2.762352 4.394290 -1.058601
C 2.347906 5.012079 0.127808
C 1.700491 4.265980 1.115574
C 1.463731 2.902075 0.916829
H 0.970287 2.326303 1.703956
H 1.382650 4.743469 2.045454
H 2.535550 6.077394 0.282647
H 3.274370 4.975982 -1.828910
H 2.863756 2.558795 -2.185256
C 3.080907 -0.288161 -0.994792
C 4.273794 0.150394 -0.393225
C 5.473830 -0.518081 -0.646607
C 5.495638 -1.628023 -1.496658
C 4.311184 -2.070932 -2.093563
C 3.106398 -1.409706 -1.841643
H 2.191290 -1.777757 -2.309448
H 4.322839 -2.937366 -2.759228
H 6.435953 -2.148467 -1.693921
H 6.396041 -0.168253 -0.176430
H 4.270697 1.017914 0.270508
C 0.434376 0.498322 -2.069335
C -0.943084 1.098133 -1.758596
P -1.787107 0.237586 -0.335148
C -3.065550 1.426207 0.213382
C -4.311476 1.538129 -0.427367
C -5.236004 2.491376 0.005599
C -4.926222 3.338931 1.075102
C -3.688840 3.231714 1.717341
C -2.763156 2.275647 1.291228
H -1.799446 2.193762 1.802898
H -3.446307 3.888614 2.556119
H -5.653485 4.081813 1.411569
H -6.203741 2.573490 -0.495247
H -4.563150 0.876824 -1.259985
C -2.697208 -1.181701 -1.053196
C -3.528053 -1.921205 -0.189737
C -4.191055 -3.059989 -0.648578
C -4.020957 -3.486695 -1.971024
C -3.192555 -2.763298 -2.831913
C -2.533764 -1.614532 -2.378917
H -1.897025 -1.066131 -3.075623
H -3.058272 -3.089218 -3.866252
H -4.535672 -4.381725 -2.328462
H -4.841728 -3.618479 0.028766
H -3.666446 -1.599356 0.846622
H -1.595040 1.096588 -2.646065
H -0.844133 2.149683 -1.445133
H 0.939344 1.059005 -2.871562
H 0.344190 -0.547632 -2.399738

^{4}5A-08
Geometry with 71 atoms:

Total energy: -2967.044812830

Cr	-0.014214	-0.563426	1.192561
C	0.156242	-2.459540	0.438712
C	1.005083	-3.406093	1.286193
H	1.104138	-4.358502	0.730778
H	2.040240	-3.025625	1.382303
C	0.429866	-3.725241	2.676719
H	0.840816	-4.685552	3.028681
C	0.718683	-2.679940	3.763638
C	0.336314	-1.233882	3.420807
C	-1.047771	-0.965901	2.888157
H	-1.549856	-0.093785	3.333941
H	-1.720710	-1.832013	2.852164
H	0.610181	-0.558862	4.248607
H	1.141407	-0.898395	2.644005
H	0.182759	-2.957403	4.686933
H	1.794676	-2.704608	4.009976
H	-0.658567	-3.884399	2.582423
H	0.568168	-2.362086	-0.581627
H	-0.880630	-2.825869	0.352038
P	-1.654119	0.211556	-0.492492
C	-2.551248	-1.179079	-1.269169
C	-2.261333	-1.649937	-2.558982
C	-2.923752	-2.776580	-3.058784
C	-3.875748	-3.437502	-2.279328
C	-4.169496	-2.970210	-0.992642
C	-3.507856	-1.851517	-0.486291
H	-3.738675	-1.495949	0.521720
H	-4.915549	-3.481993	-0.379953
H	-4.390567	-4.317252	-2.672842
H	-2.692985	-3.135827	-4.064617
H	-1.522693	-1.151641	-3.189520
C	-2.931491	1.427428	-0.009058
C	-4.013683	1.713677	-0.859716
C	-4.955855	2.675864	-0.491206
C	-4.827189	3.357617	0.724548
C	-3.755724	3.074325	1.576224
C	-2.811439	2.109585	1.213164
H	-1.990638	1.878264	1.896592
H	-3.659074	3.597175	2.530727
H	-5.569391	4.106480	1.011364
H	-5.797599	2.891736	-1.153654
H	-4.128498	1.175656	-1.804208
C	-0.687722	1.057307	-1.846184
C	0.711629	0.459916	-2.052115
P	1.672531	0.429928	-0.453403
C	3.258200	-0.395083	-0.820128
C	4.090653	-0.707311	0.270847
C	5.318002	-1.338421	0.064738
C	5.721264	-1.678177	-1.231622
C	4.895998	-1.379705	-2.318944
C	3.669325	-0.738263	-2.118805
H	3.045474	-0.508736	-2.984657
H	5.207663	-1.643484	-3.332513
H	6.679433	-2.177905	-1.393258
H	5.958853	-1.571909	0.918306
H	3.780818	-0.451092	1.288464
C	2.060263	2.201979	-0.160819
C	1.105891	2.986790	0.514144
C	1.331753	4.348532	0.729173
C	2.519875	4.937004	0.284833
C	3.477371	4.161604	-0.377447
C	3.251403	2.800756	-0.602732
H	4.006424	2.204887	-1.120811
H	4.407684	4.619359	-0.722573
H	2.701277	6.000577	0.457826
H	0.579878	4.948315	1.247789
H	0.170457	2.543525	0.868811
H	1.264159	1.041051	-2.807231
H	0.651828	-0.581849	-2.405704
H	-1.266658	1.045727	-2.782615
H	-0.614337	2.111935	-1.538240

^{45}A-09

Geometry with 71 atoms:

Total energy: -2967.044922040

Cr	-0.164873	-0.782785	1.102237
C	-0.305647	-2.637197	0.236024
C	0.179562	-3.829073	1.062847
H	0.083209	-4.736665	0.436668
H	1.261878	-3.748069	1.278899
C	-0.582795	-4.071712	2.375440
H	-0.454473	-5.123065	2.680611
C	-0.138932	-3.194539	3.554610
C	-0.137476	-1.681376	3.298826
C	-1.378627	-1.072162	2.696230
H	-1.712420	-0.143064	3.183928
H	-2.222840	-1.755011	2.538668
H	0.206641	-1.140988	4.196233
H	0.780761	-1.495011	2.606779
H	-0.800167	-3.384393	4.416826
H	0.875233	-3.497541	3.868753
H	-1.663672	-3.945039	2.190868
H	0.255292	-2.563557	-0.713009
H	-1.377603	-2.752693	-0.001160
P	-1.633782	0.266158	-0.577355
C	-3.240480	-0.500669	-0.987082
C	-3.300861	-1.629271	-1.823724
C	-4.526504	-2.253025	-2.070493
C	-5.696625	-1.763629	-1.482091
C	-5.639768	-0.644655	-0.645301
C	-4.418846	-0.013673	-0.395884
H	-4.388076	0.862776	0.255622
H	-6.551606	-0.257106	-0.184571
H	-6.653435	-2.254165	-1.676680
H	-4.565216	-3.125627	-2.727041
H	-2.398150	-2.029652	-2.288953
C	-1.961607	2.039314	-0.253148
C	-1.922826	2.506590	1.072191
C	-2.145154	3.858280	1.352937
C	-2.403499	4.753626	0.311601
C	-2.449767	4.294933	-1.010258
C	-2.235259	2.944781	-1.293723
H	-2.286008	2.602050	-2.329501
H	-2.658298	4.992677	-1.824794
H	-2.573478	5.811036	0.528502
H	-2.114862	4.210303	2.386726
H	-1.720837	1.812090	1.891294
C	-0.622988	0.231409	-2.137517
C	0.734369	0.915235	-1.926380
P	1.678843	0.204444	-0.467325
C	2.961086	-0.889556	-1.179038
C	3.207394	-2.128255	-0.565541
C	4.199452	-2.979157	-1.061875
C	4.952745	-2.598370	-2.175280
C	4.719046	-1.361561	-2.788444
C	3.731197	-0.508523	-2.293428
H	3.575169	0.462324	-2.770507
H	5.312992	-1.058461	-3.654127
H	5.726009	-3.264056	-2.566492
H	4.380363	-3.941746	-0.577531
H	2.621492	-2.432928	0.303317
C	2.577633	1.645738	0.233746
C	3.961394	1.623592	0.472879
C	4.583478	2.713003	1.091301
C	3.835604	3.827865	1.480299
C	2.454971	3.851483	1.253828
C	1.827351	2.765776	0.640658
H	0.746624	2.800059	0.478915
H	1.861417	4.717873	1.556287
H	4.327155	4.677089	1.961044
H	5.661803	2.688686	1.267060
H	4.559756	0.760678	0.173158
H	0.598923	1.989882	-1.733284
H	1.348867	0.829764	-2.834465
H	-0.488817	-0.830102	-2.400711
H	-1.178304	0.698140	-2.966073

^{45}A-10

Geometry with 71 atoms:

Total energy: -2967.042818690

Cr	0.068141	-0.529830	1.222509
C	1.423414	-0.512591	2.708208
C	0.318050	-1.140221	3.533566
H	0.065944	-0.521694	4.410912
H	-0.689923	-1.095610	2.965371
C	0.508791	-2.614203	3.938378
H	-0.066517	-2.807380	4.858480
C	0.101768	-3.665580	2.895589
C	0.689075	-3.507408	1.482754
C	-0.020275	-2.477838	0.604085
H	-1.102766	-2.700537	0.552577
H	0.383613	-2.487935	-0.422728
H	1.771203	-3.294363	1.538644
H	0.613404	-4.489387	0.977001
H	0.386941	-4.652699	3.295339
H	-1.001055	-3.684208	2.813199
H	1.570342	-2.749095	4.206547
H	1.670295	0.523206	2.993797
H	2.337926	-1.113123	2.621783
P	-1.806430	0.202117	-0.384415
C	-3.329696	-0.757692	-0.709889
C	-4.588453	-0.302684	-0.281107
C	-5.724649	-1.093359	-0.475571
C	-5.617821	-2.342149	-1.094472
C	-4.366846	-2.803682	-1.517070
C	-3.226403	-2.021399	-1.322258
H	-2.256686	-2.405064	-1.648201
H	-4.276010	-3.780116	-1.999135
H	-6.508528	-2.956329	-1.246971
H	-6.699116	-0.727384	-0.142889
H	-4.689352	0.672846	0.199640
C	-2.314198	1.939835	-0.101429
C	-1.971974	2.553824	1.115926
C	-2.290987	3.895072	1.351329
C	-2.958047	4.632840	0.370049
C	-3.310002	4.028482	-0.843131
C	-2.990568	2.690315	-1.080155
H	-3.275693	2.228152	-2.028735
H	-3.836415	4.604113	-1.608339
H	-3.208123	5.681199	0.550186
H	-2.020749	4.361315	2.301780
H	-1.458086	1.982570	1.895690
C	-0.926516	0.276158	-2.031231
C	0.384123	1.061166	-1.906795
P	1.500848	0.368962	-0.587457
C	2.494865	-0.956532	-1.356881
C	3.385816	-1.664045	-0.527827
C	4.138350	-2.719625	-1.042901
C	3.997555	-3.092809	-2.384744
C	3.107242	-2.401317	-3.209719
C	2.358140	-1.334241	-2.701765
H	1.671244	-0.808654	-3.367718
H	2.993484	-2.689444	-4.257569
H	4.581174	-3.925008	-2.785590
H	4.831690	-3.258419	-0.392697
H	3.488410	-1.388324	0.524595
C	2.639151	1.745630	-0.195705
C	2.155930	2.779837	0.626435
C	2.970233	3.870668	0.934969
C	4.276087	3.932066	0.435433
C	4.762212	2.903498	-0.376674
C	3.948744	1.811812	-0.695668
H	4.337943	1.013621	-1.331181
H	5.781563	2.949275	-0.767598
H	4.915769	4.782857	0.682303
H	2.587361	4.672167	1.571313
H	1.137170	2.740595	1.024203
H	0.184082	2.100055	-1.599190
H	0.920416	1.120534	-2.866184
H	-0.742986	-0.763025	-2.347116
H	-1.588283	0.732081	-2.784036

^{45}A-11

Geometry with 71 atoms:

Total energy: -2967.042311370

Cr	0.159191	-0.652367	1.171769
C	1.603647	-0.937291	2.598616
C	1.534446	-2.339207	3.212920
H	1.899014	-3.076419	2.476969
H	2.220423	-2.428646	4.076465
C	0.122648	-2.727804	3.675719
H	-0.129939	-2.161856	4.589993
C	-0.991357	-2.486868	2.646301
C	-0.833929	-3.173344	1.261484
C	0.170925	-2.493768	0.324048
H	-0.156128	-2.519716	-0.727132
H	1.195347	-2.884828	0.403114
H	-0.563226	-4.228109	1.448904
H	-1.823440	-3.186623	0.779016
H	-1.953696	-2.803847	3.079985
H	-1.181643	-1.377253	2.548455
H	0.102525	-3.793972	3.960155

H	1.321135	-0.165001	3.352366
H	2.626696	-0.701939	2.261210
P	-1.664328	0.269040	-0.440030
C	-2.768230	-1.045482	-1.075085
C	-2.503323	-1.732645	-2.270485
C	-3.309230	-2.808227	-2.658743
C	-4.385152	-3.205894	-1.861260
C	-4.655573	-2.524890	-0.668638
C	-3.849276	-1.456727	-0.272771
H	-4.070102	-0.934066	0.662036
H	-5.498127	-2.828423	-0.042492
H	-5.014248	-4.044869	-2.167967
H	-3.094523	-3.334462	-3.592019
H	-1.669169	-1.439809	-2.911317
C	-2.755779	1.659943	0.036697
C	-3.943690	1.954575	-0.654253
C	-4.711518	3.060874	-0.283755
C	-4.301163	3.881730	0.772996
C	-3.120010	3.595009	1.463779
C	-2.351715	2.486118	1.099228
H	-1.429387	2.268856	1.646339
H	-2.798508	4.232075	2.291215
H	-4.905664	4.745652	1.059957
H	-5.635179	3.284250	-0.823316
H	-4.272586	1.315722	-1.477409
C	-0.719144	0.938126	-1.907710
C	0.646269	0.267608	-2.108191
P	1.627109	0.284154	-0.526800
C	3.178534	-0.611000	-0.878765
C	4.408758	-0.123827	-0.404616
C	5.579521	-0.857999	-0.612057
C	5.534223	-2.080618	-1.288312
C	4.311463	-2.573075	-1.755713
C	3.136470	-1.847554	-1.548511
H	2.189691	-2.255390	-1.907900
H	4.270118	-3.529135	-2.283094
H	6.452001	-2.650790	-1.451009
H	6.531996	-0.469466	-0.243783
H	4.458986	0.831194	0.122852
C	2.065315	2.040647	-0.270682
C	2.674762	2.798699	-1.286583
C	2.970261	4.146063	-1.073514
C	2.663244	4.748683	0.152518
C	2.064923	4.000752	1.169807
C	1.768174	2.650828	0.959499
H	1.315682	2.069159	1.767253
H	1.832042	4.466096	2.130419
H	2.896260	5.803845	0.314937
H	3.444721	4.729100	-1.866482
H	2.929429	2.336101	-2.243511
H	1.220039	0.772840	-2.901119
H	0.541196	-0.786247	-2.408233
H	-1.336170	0.874286	-2.817639
H	-0.584830	2.009994	-1.691038

^{4}5A-12
Geometry with 71 atoms:
Total energy: -2967.041228870

Cr	-0.155005	-0.375573	1.250998
C	-0.218218	-2.367891	0.924824
C	0.859900	-2.780277	1.933681
H	0.622228	-3.748778	2.409542
H	1.813803	-2.920375	1.401601
C	1.105287	-1.754460	3.074891
H	1.282480	-0.714334	2.671664
C	0.072627	-1.694162	4.210717
C	-1.363840	-1.362528	3.778720
C	-1.435255	-0.164858	2.827765
H	-0.981294	0.741549	3.294775
H	-2.475366	0.101135	2.578070
H	-1.817521	-2.244228	3.292745
H	-1.968335	-1.188406	4.688870
H	0.092078	-2.658585	4.746531
H	0.413956	-0.933705	4.935112
H	2.097543	-1.958573	3.509208
H	0.028183	-2.659466	-0.108645
H	-1.228207	-2.725110	1.173659
P	1.680444	0.183269	-0.545951
C	2.909315	1.497948	-0.211199
C	2.761453	2.283680	0.944572
C	3.650267	3.330979	1.206552
C	4.695476	3.595561	0.317533
C	4.853999	2.811826	-0.831879
C	3.967622	1.766451	-1.097471
H	4.105557	1.152625	-1.991274
H	5.674863	3.015638	-1.523761
H	5.393014	4.411418	0.522177
H	3.529082	3.935180	2.108820
H	1.952168	2.078321	1.652256
C	2.645345	-1.252931	-1.143451
C	2.315963	-1.959250	-2.311533
C	3.035895	-3.104810	-2.668072
C	4.088097	-3.554076	-1.866746
C	4.422935	-2.853844	-0.701931
C	3.703664	-1.714862	-0.337812
H	3.975905	-1.175473	0.573972
H	5.248520	-3.196939	-0.073681
H	4.649544	-4.447755	-2.149333
H	2.772548	-3.644762	-3.580848
H	1.502878	-1.627525	-2.960009
C	0.712362	0.834369	-2.003019
C	-0.678665	0.201214	-2.146037
P	-1.663443	0.237937	-0.562015
C	-2.251542	1.965513	-0.388328
C	-3.566990	2.352916	-0.689557
C	-3.960198	3.683751	-0.519003
C	-3.050177	4.635186	-0.048787
C	-1.739406	4.255186	0.258869
C	-1.343796	2.926180	0.097623
H	-0.318298	2.641353	0.351887
H	-1.025343	4.992789	0.632935
H	-3.363873	5.673333	0.084406
H	-4.986710	3.976548	-0.752641
H	-4.289482	1.618355	-1.051628
C	-3.121155	-0.811951	-0.884368
C	-3.664500	-0.944662	-2.175446
C	-4.789649	-1.746456	-2.382735
C	-5.382433	-2.418045	-1.308633
C	-4.847172	-2.289075	-0.023553
C	-3.720166	-1.492090	0.190149
H	-3.302575	-1.402643	1.193539
H	-5.304999	-2.814921	0.817588
H	-6.262005	-3.044699	-1.474979
H	-5.205243	-1.845138	-3.388450
H	-3.221122	-0.422895	-3.025952
H	-0.612716	-0.862944	-2.424065
H	-1.246338	0.715000	-2.937303
H	0.624214	1.918173	-1.828221
H	1.293710	0.714293	-2.931038

^{4}5B-01
Geometry with 79 atoms:
Total energy: -3195.955323320

Cr	-0.418964	-0.758624	1.117726
C	0.979955	-1.136175	2.600316
C	0.447004	-1.662293	3.943033
C	-0.204161	-3.054343	3.883558
C	-1.647544	-3.085595	3.360366
C	-1.890295	-2.375702	2.021645
C	-0.954601	-2.699967	0.881519
H	-1.455438	-2.955305	-0.062450
H	-0.185543	-3.442177	1.127536
H	-2.949628	-2.455046	1.727911
H	-1.845491	-1.248159	2.278858
H	-2.316466	-2.639572	4.117494
H	-1.968864	-4.134808	3.244995
H	0.434016	-3.717599	3.273585
H	-0.211862	-3.498459	4.892776
H	1.281069	-1.711100	4.669026
H	-0.275084	-0.948882	4.389511
H	1.534791	-0.192158	2.754444
H	1.715533	-1.855446	2.196056
P	1.336860	-0.088861	-0.501892
C	2.373371	1.233567	0.233817
C	2.002379	2.586374	0.182144
C	2.753325	3.550461	0.862014
C	3.878348	3.175223	1.602086
C	4.251689	1.828103	1.657972
C	3.504025	0.862004	0.981591
H	3.804200	-0.186975	1.034066
H	5.130966	1.525827	2.232195
H	4.464920	3.930285	2.131126
H	2.455886	4.600832	0.807392
H	1.127125	2.909909	-0.383551
C	2.491856	-1.361888	-1.107427
C	2.342815	-2.699846	-0.716847
C	3.234622	-3.680489	-1.158995
C	4.291175	-3.315938	-1.995646
C	4.462180	-1.988643	-2.402209
C	3.561840	-1.005282	-1.968650
O	3.633561	0.296990	-2.320842
C	4.755464	0.782662	-3.042327
H	4.809714	0.345121	-4.054135
H	5.697412	0.581483	-2.503968
H	4.616722	1.868578	-3.128006
H	5.292032	-1.728397	-3.058967
H	4.999428	-4.072038	-2.343890
H	3.106951	-4.718492	-0.845613
H	1.520083	-2.969136	-0.054701
C	0.532110	0.630437	-2.027631
C	-0.831439	-0.010108	-2.309412
P	-1.893602	0.051617	-0.781974
C	-3.556681	-0.506332	-1.282130
C	-4.672909	-0.107246	-0.523605
C	-5.944892	-0.588993	-0.836754
C	-6.117604	-1.479677	-1.902323
C	-5.012246	-1.885816	-2.654464
C	-3.735431	-1.405235	-2.347841
H	-2.886033	-1.736506	-2.948816
H	-5.140900	-2.580352	-3.488220
H	-7.114095	-1.855998	-2.145612
H	-6.806312	-0.266322	-0.246791
H	-4.550663	0.591984	0.307973
C	-2.026869	1.847338	-0.448192
C	-2.659043	2.723226	-1.345353
C	-2.684489	4.098009	-1.113835
C	-2.061591	4.607097	0.028800
C	-1.429461	3.757968	0.940546
C	-1.416958	2.374934	0.710296
O	-0.805634	1.492594	1.585128
C	-0.354973	2.005170	2.853318
H	0.521492	2.655974	2.716856
H	-1.169762	2.548296	3.355481
H	-0.072499	1.140336	3.459529
H	-0.945315	4.186224	1.816111
H	-2.063877	5.682566	0.221692
H	-3.181236	4.766947	-1.819448
H	-3.141738	2.312429	-2.236292
H	-0.714100	-1.072731	-2.578036
H	-1.336331	0.494409	-3.148454
H	1.220032	0.503361	-2.874499
H	0.415899	1.712037	-1.871180

^{4}5B-02
Geometry with 79 atoms:
Total energy: -3195.956956440

Cr	-0.214737	-0.628303	0.853507
C	0.054614	-2.528914	0.098955
C	0.982135	-3.428895	0.926994
C	0.443930	-3.815903	2.315121
C	0.614554	-2.757571	3.415012
C	0.105927	-1.349658	3.074516
C	-1.277154	-1.222066	2.483065
H	-1.892099	-0.427181	2.928017
H	-1.837462	-2.160595	2.395872
H	0.267013	-0.670185	3.928763
H	0.907394	-0.931117	2.346516
H	1.683814	-2.684756	3.682849
H	0.090632	-3.094017	4.325688
H	-0.621259	-4.088831	2.218302
H	0.953214	-4.730910	2.661056
H	1.164050	-4.364147	0.364197
H	1.979436	-2.961831	1.033554
H	0.442214	-2.452715	-0.933301
H	-0.949347	-2.985703	0.028406
P	-1.899286	0.015597	-0.732836
C	-3.272010	-1.104184	-1.154164
C	-3.269934	-1.851307	-2.342905
C	-4.277112	-2.791242	-2.582033
C	-5.287160	-2.995021	-1.638463
C	-5.285542	-2.261933	-0.446216
C	-4.280462	-1.326271	-0.198344
H	-4.280674	-0.766399	0.739809

H	-6.070321	-2.421688	0.297135
H	-6.074634	-3.728083	-1.829113
H	-4.269454	-3.365618	-3.511475
H	-2.485112	-1.714211	-3.089951
C	-2.624263	1.504877	0.048165
C	-3.848877	2.062873	-0.345117
C	-4.345772	3.208605	0.279826
C	-3.611843	3.802625	1.308934
C	-2.387018	3.266472	1.720092
C	-1.893395	2.119620	1.090142
O	-0.686538	1.543772	1.431639
C	0.167646	2.191572	2.382563
H	1.109973	1.630295	2.381524
H	-0.280679	2.169662	3.388274
H	0.376178	3.227179	2.076683
H	-1.836427	3.744478	2.529125
H	-3.993464	4.695911	1.809046
H	-5.302007	3.632603	-0.033253
H	-4.422544	1.584196	-1.142461
C	-1.107655	0.626586	-2.320734
C	0.346711	0.152823	-2.489191
P	1.354728	0.319175	-0.923752
C	1.911768	2.072737	-0.870540
C	3.274312	2.411705	-0.817031
C	3.668275	3.749036	-0.711250
C	2.711616	4.766608	-0.662020
C	1.352655	4.439812	-0.717398
C	0.954739	3.104395	-0.811867
H	-0.111951	2.879475	-0.836860
H	0.595065	5.226948	-0.683213
H	3.023187	5.811001	-0.583341
H	4.732484	3.994935	-0.673315
H	4.037378	1.632859	-0.865503
C	2.859525	-0.671576	-1.222437
C	3.231620	-1.167702	-2.479521
C	4.354802	-1.986673	-2.625497
C	5.117081	-2.314284	-1.503123
C	4.773509	-1.827482	-0.238163
C	3.650111	-1.002829	-0.095157
O	3.249192	-0.466150	1.087127
C	3.951417	-0.776208	2.280395
H	3.947808	-1.859973	2.485512
H	4.993289	-0.414516	2.241111
H	3.427594	-0.256159	3.093505
H	5.382995	-2.093019	0.625224
H	5.995232	-2.956450	-1.605540
H	4.630204	-2.365317	-3.611895
H	2.643627	-0.916647	-3.364225
H	0.827850	0.691185	-3.320209
H	0.366106	-0.922171	-2.728738
H	-1.163226	1.723589	-2.285305
H	-1.717726	0.320860	-3.183616

^{4}5B-03
Geometry with 79 atoms:
Total energy: -3195.958416660

Cr	-0.264470	-0.442652	1.046722
C	-0.199874	-2.416330	0.459185
C	0.705625	-3.337120	1.285975
C	0.264622	-3.547696	2.743022
C	0.635542	-2.417538	3.713674
C	0.207432	-1.004320	3.292170
C	-1.208405	-0.812630	2.809061
H	-1.719249	0.068161	3.224065
H	-1.842366	-1.705254	2.863898
H	0.497399	-0.273916	4.066309
H	0.968174	-0.716050	2.461312
H	1.729668	-2.418122	3.867287
H	0.184481	-2.623617	4.699205
H	-0.825393	-3.720684	2.764548
H	0.718776	-4.474322	3.132322
H	0.740496	-4.328585	0.795668
H	1.746284	-2.968236	1.266958
H	0.120669	-2.433475	-0.598356
H	-1.239693	-2.788979	0.489381
P	-1.940362	0.051974	-0.605680
C	-3.460783	-0.923248	-0.819971
C	-3.934687	-1.339612	-2.074432
C	-5.102959	-2.103666	-2.160457
C	-5.802301	-2.452434	-1.002069
C	-5.330895	-2.042120	0.250490
C	-4.161638	-1.286854	0.344548
H	-3.784169	-0.981834	1.324091
H	-5.872194	-2.319512	1.158212
H	-6.714510	-3.049708	-1.073827
H	-5.466619	-2.426461	-3.139004
H	-3.404035	-1.076848	-2.991339
C	-2.448132	1.773084	-0.245923
C	-3.527038	2.387259	-0.897534
C	-3.876583	3.708171	-0.614139
C	-3.138906	4.421701	0.333486
C	-2.062184	3.830468	1.001561
C	-1.716185	2.504248	0.714523
O	-0.662928	1.859820	1.333421
C	0.019210	2.525603	2.401939
H	0.769901	1.822964	2.780074
H	-0.680213	2.781079	3.213418
H	0.530901	3.428701	2.037250
H	-1.507661	4.412367	1.736313
H	-3.401400	5.456579	0.565789
H	-4.720241	4.175681	-1.125839
H	-4.104718	1.814195	-1.627687
C	-1.099870	0.152923	-2.259631
C	0.190938	0.978399	-2.156275
P	1.326986	0.375688	-0.807707
C	2.493450	1.773047	-0.554855
C	3.015710	1.994163	0.729827
C	3.900240	3.049809	0.964350
C	4.270367	3.897944	-0.084183
C	3.758862	3.682204	-1.367774
C	2.878175	2.623250	-1.605222
H	2.500289	2.464215	-2.617671
H	4.050590	4.338643	-2.191322
H	4.960432	4.725489	0.098051
H	4.302682	3.210157	1.967805
H	2.736283	1.327887	1.547957
C	2.317214	-0.965125	-1.562695
C	2.150238	-1.440762	-2.868826
C	2.898806	-2.526547	-3.335854
C	3.821466	-3.142270	-2.488854
C	4.002859	-2.689645	-1.177515
C	3.248799	-1.606394	-0.712126
O	3.330616	-1.099657	0.545384
C	4.291749	-1.605363	1.457146
H	5.317732	-1.477734	1.071762
H	4.181762	-1.019526	2.379811
H	4.115984	-2.670154	1.687495
H	4.724412	-3.186082	-0.528801
H	4.411454	-3.989954	-2.845747
H	2.760208	-2.886458	-4.357447
H	1.428706	-0.969553	-3.539471
H	-0.046369	2.020661	-1.888039
H	0.705265	1.014121	-3.128041
H	-1.779442	0.599982	-3.002340
H	-0.893038	-0.883975	-2.570768

^{4}5B-04
Geometry with 79 atoms:
Total energy: -3195.957504030

Cr	-0.062737	-0.497251	1.169183
C	-1.120567	-1.504197	2.581487
C	0.259420	-1.818079	3.097351
C	0.652408	-1.255365	4.469506
C	0.368679	0.239473	4.671396
C	0.930745	1.157551	3.575095
C	0.118825	1.218330	2.277443
H	0.570730	1.935817	1.576784
H	-0.911891	1.562045	2.480087
H	1.001405	2.180742	3.991896
H	1.978267	0.864756	3.364214
H	0.794098	0.529575	5.646376
H	-0.718185	0.411840	4.758317
H	0.114115	-1.836635	5.237320
H	1.727889	-1.445356	4.633588
H	0.499686	-2.892399	3.034240
H	1.075437	-1.404485	2.376695
H	-1.686135	-2.374600	2.227673
H	-1.735498	-0.883034	3.243972
P	-1.640511	0.275652	-0.603454
C	-3.136675	-0.780991	-0.713731
C	-3.603071	-1.336081	-1.917087
C	-4.737777	-2.153828	-1.921735
C	-5.423342	-2.415299	-0.732039
C	-4.974101	-1.853226	0.467986
C	-3.835161	-1.045661	0.479146
H	-3.483112	-0.619261	1.420714
H	-5.508310	-2.049165	1.400858
H	-6.309576	-3.054549	-0.739878
H	-5.089306	-2.583756	-2.862861
H	-3.096248	-1.135518	-2.862383
C	-2.301680	1.990141	-0.657990
C	-3.681798	2.239972	-0.719913
C	-4.183236	3.543791	-0.695681
C	-3.298332	4.618152	-0.604376
C	-1.919276	4.399322	-0.545622
C	-1.415662	3.091883	-0.577042
O	-0.090422	2.802432	-0.548171
C	0.857688	3.842458	-0.345084
H	1.840029	3.358383	-0.287513
H	0.665090	4.380853	0.597577
H	0.856401	4.556926	-1.185753
H	-1.242447	5.250396	-0.479843
H	-3.677089	5.642856	-0.579677
H	-5.260697	3.713598	-0.745046
H	-4.380746	1.404805	-0.783323
C	-0.732880	-0.042053	-2.209832
C	0.731818	0.417609	-2.221325
P	1.646939	-0.084615	-0.673955
C	3.136260	0.965431	-0.625812
C	3.713079	1.225850	0.629400
C	4.838407	2.047029	0.731832
C	5.391565	2.622495	-0.416632
C	4.821569	2.370251	-1.669074
C	3.699801	1.543696	-1.777156
H	3.268001	1.356431	-2.762650
H	5.252960	2.818427	-2.567455
H	6.267181	3.271236	-0.336078
H	5.278235	2.245132	1.712227
H	3.272218	0.796597	1.532212
C	2.233559	-1.788032	-1.038983
C	3.491105	-2.083237	-1.581156
C	3.877622	-3.406233	-1.813316
C	3.000029	-4.444446	-1.498452
C	1.740478	-4.175710	-0.950054
C	1.362390	-2.850248	-0.717524
O	0.138624	-2.505365	-0.163359
C	-0.895585	-3.500541	-0.140178
H	-0.674178	-4.282832	0.602124
H	-1.820826	-2.986857	0.134905
H	-1.014616	-3.950122	-1.137805
H	1.076917	-5.003709	-0.703764
H	3.292083	-5.482735	-1.672811
H	4.860869	-3.622498	-2.236270
H	4.176712	-1.266893	-1.819531
H	0.790842	1.511839	-2.269123
H	1.243916	0.004242	-3.103579
H	-1.283636	0.422475	-3.042000
H	-0.784763	-1.133883	-2.346534

^{4}5B-05
Geometry with 79 atoms:
Total energy: -3195.957047090

Cr	-0.233158	-0.570031	0.887685
C	0.029413	-2.484647	0.164102
C	0.965614	-3.375928	0.991192
C	0.448320	-3.740278	2.393013
C	0.633559	-2.662839	3.471535
C	0.115429	-1.262466	3.114089
C	-1.274830	-1.152073	2.535208
H	-1.891009	-0.355376	2.975207
H	-1.829732	-2.095494	2.469565
H	0.281865	-0.569739	3.956631
H	0.907956	-0.852880	2.371277
H	1.706625	-2.582543	3.721281
H	0.124610	-2.984423	4.395985
H	-0.617762	-4.016251	2.316995
H	0.964246	-4.648570	2.746769
H	1.134332	-4.320101	0.439240
H	1.966329	-2.912307	1.075515
H	0.400983	-2.424591	-0.874976
H	-0.977206	-2.937997	0.114613
P	-1.900197	0.035607	-0.736066
C	-3.210155	-1.131496	-1.220565

C -3.162822 -1.825417 -2.440385
C -4.122045 -2.801225 -2.728672
C -5.128875 -3.092644 -1.804952
C -5.172645 -2.411606 -0.582846
C -4.215153 -1.441351 -0.285427
H -4.249690 -0.921598 0.675259
H -5.955164 -2.639914 0.144754
H -5.878254 -3.853971 -2.034308
H -4.079636 -3.334977 -3.681102
H -2.379718 -1.618648 -3.173324
C -2.705600 1.483955 0.040852
C -3.955304 1.980314 -0.354450
C -4.518407 3.087616 0.283988
C -3.826436 3.703582 1.328802
C -2.577086 3.228270 1.742441
C -2.017029 2.121287 1.098101
O -0.781853 1.605358 1.438035
C 0.024402 2.271348 2.417167
H 0.995613 1.760737 2.413779
H -0.434681 2.200178 3.415755
H 0.180652 3.324967 2.142808
H -2.060780 3.721882 2.564646
H -4.260367 4.566314 1.839780
H -5.493683 3.464263 -0.030926
H -4.496146 1.483523 -1.163466
C -1.073259 0.685208 -2.287420
C 0.361782 0.158241 -2.460774
P 1.368432 0.326514 -0.893787
C 1.975941 2.064253 -0.904283
C 1.059846 3.114642 -0.705242
C 1.492711 4.442595 -0.692962
C 2.849293 4.740729 -0.857672
C 3.767694 3.703373 -1.042107
C 3.336601 2.373677 -1.068580
H 4.066239 1.576276 -1.222410
H 4.829365 3.928133 -1.171746
H 3.189414 5.779005 -0.841409
H 0.766334 5.246358 -0.547770
H 0.001727 2.902665 -0.550650
C 2.849515 -0.705751 -1.162423
C 3.208701 -1.252096 -2.402189
C 4.322075 -2.088540 -2.523607
C 5.087992 -2.380746 -1.394026
C 4.757160 -1.842968 -0.146255
C 3.641852 -1.003687 -0.026897
O 3.247749 -0.426537 1.138287
C 3.958775 -0.694951 2.336417
H 5.001170 -0.337797 2.275508
H 3.442846 -0.144178 3.134257
H 3.954457 -1.770641 2.580451
H 5.369212 -2.082551 0.722816
H 5.959082 -3.035260 -1.476925
H 4.587392 -2.507386 -3.496426
H 2.618940 -1.025935 -3.292542
H 0.858414 0.675056 -3.296302
H 0.347104 -0.918700 -2.691867
H -1.079809 1.780912 -2.196253
H -1.688334 0.449629 -3.168763

^{4}5B-06
Geometry with 79 atoms:
Total energy: -3195.959050310
Cr -0.257772 -0.525543 1.006769
C -0.116569 -2.467118 0.319796
C 0.778134 -3.408987 1.135232
C 0.281394 -3.708847 2.558561
C 0.584819 -2.626146 3.603422
C 0.148935 -1.200536 3.236264
C -1.252433 -1.006490 2.709105
H -1.795005 -0.162492 3.159107
H -1.873239 -1.909857 2.683779
H 0.392738 -0.508012 4.059588
H 0.934786 -0.856111 2.453892
H 1.670312 -2.615318 3.808587
H 0.092922 -2.892143 4.554417
H -0.804373 -3.904781 2.523165
H 0.739786 -4.646183 2.915953
H 0.861388 -4.371158 0.594876
H 1.808866 -3.014937 1.180148
H 0.248081 -2.421845 -0.722691
H -1.144777 -2.871202 0.286514
P -1.906384 -0.017366 -0.653130
C -3.440801 -0.968983 -0.877529
C -3.703059 -1.720272 -2.034269
C -4.874790 -2.479314 -2.122984
C -5.786219 -2.493586 -1.064497
C -5.525130 -1.749970 0.092808
C -4.356110 -0.995853 0.191184
H -4.152833 -0.423521 1.100454
H -6.234246 -1.761761 0.924063
H -6.701019 -3.086537 -1.138300
H -5.074381 -3.060115 -3.026741
H -3.004029 -1.723341 -2.872806
C -2.406786 1.704363 -0.283872
C -3.437096 2.350146 -0.983242
C -3.801244 3.661327 -0.674768
C -3.131442 4.333688 0.350338
C -2.104064 3.712109 1.066696
C -1.738110 2.398116 0.749162
O -0.715354 1.736892 1.398924
C -0.113161 2.339034 2.551935
H -0.859758 2.487937 3.347564
H 0.367483 3.293948 2.294407
H 0.661304 1.644476 2.898296
H -1.603452 4.259366 1.864184
H -3.409574 5.358880 0.606076
H -4.606134 4.152366 -1.225312
H -3.967273 1.807860 -1.770782
C -1.046022 0.056862 -2.298963
C 0.220976 0.918038 -2.206548
P 1.353862 0.426275 -0.802313
C 2.388013 1.930498 -0.569220
C 1.750259 3.148248 -0.266404
C 2.498191 4.305378 -0.038247
C 3.894916 4.261706 -0.097398
C 4.535612 3.056354 -0.396949
C 3.790293 1.897314 -0.633518
H 4.309681 0.969992 -0.878506
H 5.626179 3.015564 -0.455043
H 4.480981 5.166020 0.083491
H 1.986042 5.245104 0.184096
H 0.661275 3.205214 -0.218777
C 2.463697 -0.866370 -1.465376
C 2.415084 -1.345401 -2.780639
C 3.227044 -2.408076 -3.189282
C 4.100219 -2.997994 -2.274274
C 4.170655 -2.539332 -0.954885
C 3.350343 -1.480251 -0.547095
O 3.339004 -0.962693 0.707622
C 4.213612 -1.473150 1.701183
H 5.270740 -1.330321 1.418378
H 4.009044 -0.900056 2.615483
H 4.029638 -2.543144 1.897630
H 4.859790 -3.012293 -0.255404
H 4.740022 -3.827837 -2.584226
H 3.177044 -2.769058 -4.218535
H 1.737071 -0.891402 -3.505496
H -0.055245 1.963549 -2.001163
H 0.766082 0.928926 -3.162329
H -1.731321 0.454259 -3.064570
H -0.804408 -0.983276 -2.570977

^{4}5B-07
Geometry with 79 atoms:
Total energy: -3195.957233990
Cr -0.178855 -0.686444 0.853239
C 0.177992 -2.541839 0.016556
C 1.173718 -3.434269 0.769708
C 0.715456 -3.892795 2.163841
C 0.894182 -2.864862 3.290290
C 0.308728 -1.471898 3.019874
C -1.112718 -1.394162 2.516840
H -1.738126 -0.644878 3.022541
H -1.629367 -2.358926 2.448373
H 0.491950 -0.807365 3.881182
H 1.046985 -1.005806 2.256912
H 1.971234 -2.752445 3.507658
H 0.431736 -3.252375 4.213895
H -0.340765 -4.208344 2.104578
H 1.276962 -4.796653 2.453695
H 1.363954 -4.339982 0.163207
H 2.156630 -2.934447 0.850108
H 0.526032 -2.401637 -1.022771
H -0.802448 -3.047276 -0.047968
P 1.331616 0.381445 -0.912742
C 1.897310 2.133277 -0.844438
C 0.963477 3.157256 -0.593464
C 1.372553 4.491222 -0.525920
C 2.721715 4.822536 -0.687228
C 3.657280 3.811775 -0.924109
C 3.250380 2.476830 -1.005688
H 3.993797 1.702099 -1.202258
H 4.713448 4.061518 -1.052928
H 3.042401 5.865481 -0.628656
H 0.632361 5.273808 -0.340671
H -0.091217 2.925798 -0.442542
C 2.828310 -0.593831 -1.289692
C 3.150552 -1.071596 -2.566932
C 4.281614 -1.866723 -2.773140
C 5.103119 -2.185872 -1.691061
C 4.808810 -1.717428 -0.406720
C 3.674577 -0.921144 -0.202757
O 3.309915 -0.414370 1.004447
C 4.079643 -0.714988 2.157988
H 3.580584 -0.221933 3.002762
H 5.106184 -0.319264 2.072133
H 4.121648 -1.800786 2.348153
H 5.464701 -1.976476 0.423773
H 5.989563 -2.807066 -1.840674
H 4.517186 -2.232282 -3.774643
H 2.517063 -0.823975 -3.420289
C 0.272578 0.274946 -2.447546
C -1.168036 0.757378 -2.208942
P -1.934421 -0.004859 -0.672662
C -3.307704 -1.082905 -1.198556
C -3.647787 -2.153645 -0.353078
C -4.716559 -2.991869 -0.677847
C -5.449551 -2.772353 -1.848314
C -5.114644 -1.710187 -2.694337
C -4.048623 -0.865689 -2.373277
H -3.807889 -0.036274 -3.042510
H -5.686576 -1.535627 -3.608860
H -6.282904 -3.431418 -2.103732
H -4.973505 -3.822863 -0.016675
H -3.072644 -2.327254 0.558582
C -2.700354 1.395431 0.236364
C -3.979550 1.892934 -0.044342
C -4.513243 2.952590 0.693395
C -3.765635 3.515538 1.729159
C -2.490391 3.029668 2.038357
C -1.961415 1.972328 1.292943
O -0.707979 1.443292 1.535231
C 0.150046 2.066501 2.498417
H 0.278496 3.134814 2.271677
H -0.247624 1.937192 3.517055
H 1.124190 1.570336 2.410676
H -1.930781 3.472961 2.860914
H -4.176310 4.339739 2.317043
H -5.511656 3.330389 0.464017
H -4.569451 1.435724 -0.842004
H -1.786575 0.519224 -3.086174
H -1.209588 1.848734 -2.083709
H 0.263445 -0.789664 -2.729367
H 0.731004 0.838752 -3.274681

^{4}5B-08
Geometry with 79 atoms:
Total energy: -3195.957222610
Cr -0.171147 -0.693424 0.851865
C 0.188041 -2.548196 0.015104
C 1.188697 -3.436297 0.767266
C 0.735469 -3.894080 2.163428
C 0.914884 -2.864283 3.288143
C 0.324367 -1.473399 3.018027
C -1.098855 -1.400536 2.519154
H -1.724737 -0.652019 3.025377
H -1.612749 -2.367002 2.454303
H 0.508427 -0.806965 3.877694
H 1.059129 -1.006506 2.252247
H 1.992318 -2.748495 3.501747
H 0.456786 -3.252130 4.213791
H -0.320165 -4.212199 2.107627
H 1.299878 -4.796251 2.452886

H 1.380369 -4.342362 0.161739
H 2.170116 -2.933083 0.844703
H 0.533401 -2.407519 -1.025144
H -0.790647 -3.057402 -0.046863
P -1.931453 -0.018230 -0.671412
C -3.305447 -1.099373 -1.188327
C -4.051313 -0.887403 -2.360880
C -5.118239 -1.733788 -2.673815
C -5.449152 -2.792408 -1.821805
C -4.711269 -3.006582 -0.653476
C -3.641572 -2.166517 -0.336731
H -3.062771 -2.335794 0.573432
H -4.965143 -3.834765 0.012392
H -6.283394 -3.452803 -2.070820
H -5.694187 -1.563469 -3.586606
H -3.813779 -0.060780 -3.034604
C -2.696388 1.385230 0.233508
C -3.975642 1.881756 -0.048508
C -4.508428 2.945123 0.684422
C -3.759846 3.512710 1.716997
C -2.484800 3.027457 2.027839
C -1.956710 1.966331 1.287122
O -0.704102 1.437338 1.532147
C 0.159458 2.072462 2.482786
H 1.134299 1.578267 2.392709
H -0.230241 1.951803 3.505583
H 0.283022 3.138688 2.244162
H -1.924358 3.474011 2.848044
H -4.169817 4.339864 2.301224
H -5.506802 3.322251 0.453765
H -4.566275 1.420877 -0.843626
C -1.170781 0.740569 -2.213137
C 0.273156 0.268557 -2.450620
P 1.331246 0.380356 -0.915873
C 1.868808 2.140116 -0.835378
C 3.221687 2.504632 -0.940629
C 3.603583 3.846119 -0.844613
C 2.643359 4.842295 -0.648613
C 1.294000 4.489849 -0.542400
C 0.909459 3.149585 -0.624667
H -0.146969 2.901736 -0.517604
H 0.534191 5.260603 -0.389803
H 2.944862 5.890300 -0.579362
H 4.660061 4.112455 -0.930392
H 3.985210 1.742242 -1.105190
C 2.839138 -0.573610 -1.301637
C 3.167868 -1.028349 -2.585819
C 4.305768 -1.810600 -2.802463
C 5.127839 -2.140091 -1.723880
C 4.827413 -1.694207 -0.433054
C 3.686490 -0.910291 -0.218572
O 3.317395 -0.424022 0.995706
C 4.091207 -0.732650 2.144585
H 4.140692 -1.820263 2.322023
H 5.114974 -0.329209 2.061513
H 3.590184 -0.252506 2.995582
H 5.483848 -1.960640 0.394580
H 6.019602 -2.751632 -1.881510
H 4.546188 -2.158185 -3.809199
H 2.534048 -0.772634 -3.436536
H 0.727522 0.836772 -3.277005
H 0.272615 -0.795794 -2.733304
H -1.220907 1.832195 -2.095805
H -1.787993 0.491328 -3.088201

^{45}5B-09
Geometry with 79 atoms:
Total energy: -3195.956866690
Cr 0.134687 -0.836409 -0.758184
C -0.207813 -2.642760 0.174702
C -1.233231 -3.552521 -0.516881
C -0.811303 -4.075339 -1.900249
C -1.013564 -3.099684 -3.068748
C -0.415440 -1.698742 -2.880871
C 1.019813 -1.605789 -2.421322
H 1.629384 -0.875822 -2.972249
H 1.535395 -2.569818 -2.334576
H -0.617464 -1.074803 -3.767982
H -1.126694 -1.187656 -2.122986
H -2.095238 -2.992341 -3.264457
H -0.576723 -3.533599 -3.984115
H 0.245032 -4.392350 -1.852578
H -1.382590 -4.988889 -2.135493
H -1.423658 -4.429188 0.130806
H -2.210700 -3.040423 -0.597754
H -0.531327 -2.447112 1.213645
H 0.766973 -3.159754 0.241845
P 1.938640 -0.080921 0.660113
C 3.440534 -1.048375 1.029917
C 4.292682 -0.752764 2.109077
C 5.445827 -1.513006 2.318948
C 5.757105 -2.570298 1.457588
C 4.913288 -2.868134 0.383431
C 3.757988 -2.112650 0.168637
H 3.096859 -2.348027 -0.667382
H 5.151218 -3.696170 -0.288509
H 6.658538 -3.164347 1.626713
H 6.103750 -1.277511 3.158964
H 4.069478 0.071283 2.790982
C 2.507897 1.408220 -0.263871
C 3.724461 2.051247 0.005762
C 4.118836 3.178237 -0.718211
C 3.292356 3.667603 -1.731787
C 2.078839 3.040477 -2.029433
C 1.689711 1.913439 -1.298883
O 0.501901 1.254044 -1.538465
C -0.478919 1.834424 -2.409417
H -1.393425 1.242813 -2.276918
H -0.145354 1.784123 -3.457585
H -0.688165 2.873788 -2.118583
H 1.452445 3.432833 -2.829653
H 3.592256 4.545303 -2.309210
H 5.069602 3.666757 -0.495561
H 4.377525 1.657612 0.787760
C 1.278772 0.562900 2.302810
C -0.216854 0.262532 2.531433
P -1.268099 0.380891 0.997145
C -1.696354 2.156891 0.787597
C -3.017160 2.567128 0.537871
C -3.304703 3.910031 0.276721
C -2.282104 4.863113 0.263220
C -0.965271 4.465323 0.516183
C -0.673385 3.123608 0.771539
H 0.364679 2.842028 0.946676
H -0.156719 5.200582 0.511186
H -2.510539 5.912366 0.060833
H -4.338056 4.212194 0.088672
H -3.831526 1.841168 0.553021
C -2.835241 -0.459811 1.402640
C -3.220982 -0.810987 2.703378
C -4.403515 -1.518975 2.934555
C -5.212049 -1.876874 1.854736
C -4.854838 -1.532063 0.547329
C -3.668616 -0.823984 0.317728
O -3.245442 -0.431916 -0.916483
C -4.018860 -0.759901 -2.061288
H -4.138446 -1.850383 -2.172627
H -5.014071 -0.284954 -2.023832
H -3.472364 -0.367951 -2.929175
H -5.503133 -1.818159 -0.280103
H -6.138903 -2.430234 2.024436
H -4.690283 -1.785650 3.953807
H -2.597596 -0.530178 3.554477
H -0.613353 0.907232 3.330585
H -0.331662 -0.782588 2.857993
H 1.483253 1.642032 2.346309
H 1.861908 0.097941 3.110712

^{45}5B-10
Geometry with 79 atoms:
Total energy: -3195.956630030
Cr 0.121650 -0.404713 1.168048
C -0.391936 0.963175 2.566105
C -1.174725 -0.187997 3.146236
C -0.751641 -0.740373 4.513113
C 0.740720 -1.060300 4.670793
C 1.341489 -1.937306 3.561295
C 1.699078 -1.189462 2.268162
H 2.234876 -1.876020 1.587231
H 2.392166 -0.361464 2.502198
H 2.255206 -2.414593 3.964340
H 0.652586 -2.779500 3.347499
H 0.869954 -1.558242 5.646149
H 1.322919 -0.124584 4.735598
H -1.049367 -0.002077 5.277066
H -1.340424 -1.651988 4.719027
H -2.260768 0.002163 3.133268
H -1.129249 -1.099893 2.433750
H -1.012197 1.789567 2.199922
H 0.437455 1.328220 3.184696
P 1.602488 0.159463 -0.730900
C 3.144249 1.126981 -0.636124
C 3.337726 2.309595 -1.369999
C 4.516913 3.045700 -1.216244
C 5.509167 2.610543 -0.334082
C 5.322053 1.432805 0.398551
C 4.146448 0.695290 0.253722
H 4.009551 -0.222117 0.829364
H 6.095190 1.086518 1.088597
H 6.429826 3.187356 -0.217559
H 4.659564 3.962228 -1.793858
H 2.577858 2.670761 -2.064937
C 2.098476 -1.529913 -1.258900
C 3.253572 -1.784590 -2.010371
C 3.590289 -3.086567 -2.388428
C 2.764880 -4.146741 -2.010520
C 1.606257 -3.919971 -1.259986
C 1.274054 -2.613990 -0.888695
O 0.144773 -2.312329 -0.148886
C -0.762414 -3.367680 0.199682
H -1.607937 -2.893919 0.710577
H -0.278966 -4.093654 0.871501
H -1.135890 -3.872297 -0.704258
H 0.982771 -4.764241 -0.969236
H 3.020677 -5.170343 -2.294169
H 4.495643 -3.270876 -2.970336
H 3.903403 -0.952332 -2.291375
C 0.651015 0.789820 -2.198283
C -0.736136 0.137819 -2.262038
P -1.647834 0.271711 -0.639495
C -3.096999 -0.833777 -0.820551
C -3.832020 -1.114020 0.347335
C -4.921619 -1.985431 0.310245
C -5.283990 -2.600781 -0.893628
C -4.560068 -2.329681 -2.057819
C -3.474449 -1.447180 -2.026198
H -2.933470 -1.242785 -2.952029
H -4.843360 -2.803076 -3.001204
H -6.131840 -3.289477 -0.923300
H -5.486157 -2.189557 1.223408
H -3.549916 -0.642917 1.293147
C -2.349432 1.969152 -0.626821
C -3.696129 2.233156 -0.917723
C -4.207736 3.531241 -0.839663
C -3.367673 4.580729 -0.462273
C -2.020817 4.346153 -0.169497
C -1.506665 3.045585 -0.257635
O -0.205002 2.734861 -0.021416
C 0.636686 3.642549 0.675988
H 1.542962 3.082627 0.938670
H 0.915722 4.502035 0.042876
H 0.156418 4.006578 1.599050
H -1.376666 5.178184 0.115620
H -3.758073 5.599190 -0.395028
H -5.258906 3.718203 -1.069085
H -4.357347 1.410816 -1.198896
H -0.642718 -0.938916 -2.477347
H -1.333759 0.590238 -3.067799
H 1.224699 0.580582 -3.114440
H 0.558291 1.877669 -2.087998

^{45}5B-11
Geometry with 79 atoms:
Total energy: -3195.953351470
Cr -0.472525 -0.065310 1.330290
C 0.056273 0.422026 3.240449
C -1.423864 0.669972 3.354391
C -2.255422 -0.232042 4.275508
C -2.059780 -1.742215 4.077667
C -2.172971 -2.241517 2.626967
C -0.917230 -2.020530 1.775578
H -1.001429 -2.555727 0.812429
H -0.039436 -2.426578 2.307974

H -2.387331 -3.326629 2.659948
H -3.061177 -1.792078 2.142172
H -2.810314 -2.255976 4.700802
H -1.079033 -2.050630 4.480267
H -2.014530 0.034072 5.318646
H -3.322102 0.015482 4.130946
H -1.656799 1.731893 3.538621
H -1.945742 0.548118 2.319494
H 0.682241 1.312359 3.382357
H 0.437162 -0.421147 3.830008
P 1.539004 -0.259896 -0.170216
C 2.757868 1.060674 0.204044
C 3.294975 1.078514 1.502703
C 4.194273 2.077451 1.882529
C 4.558948 3.074742 0.971772
C 4.031270 3.059518 -0.323312
C 3.138952 2.054971 -0.710233
H 2.755166 2.051965 -1.731494
H 4.321079 3.830633 -1.041603
H 5.256625 3.861076 1.270030
H 4.606028 2.079945 2.894708
H 3.001309 0.312459 2.225504
C 2.525766 -1.786425 -0.372568
C 2.243995 -2.919636 0.403514
C 3.013676 -4.080683 0.293026
C 4.085417 -4.107643 -0.600075
C 4.391631 -2.992062 -1.385648
C 3.614897 -1.829581 -1.282654
O 3.834217 -0.712049 -2.012334
C 4.988556 -0.609110 -2.831552
H 4.980536 0.407280 -3.246995
H 4.965994 -1.337180 -3.660779
H 5.912485 -0.749509 -2.245231
H 5.233437 -3.035905 -2.076343
H 4.699058 -5.007229 -0.693171
H 2.777466 -4.953212 0.905422
H 1.412737 -2.892663 1.106204
C 0.856741 0.128025 -1.863371
C -0.470192 -0.597173 -2.125174
P -1.725115 -0.108330 -0.844619
C -3.261548 -1.012643 -1.218095
C -4.376095 -0.778211 -0.390760
C -5.569750 -1.467327 -0.604752
C -5.659985 -2.410125 -1.635736
C -4.554544 -2.655199 -2.453759
C -3.357955 -1.958946 -2.251048
H -2.509777 -2.163109 -2.906888
H -4.620499 -3.390671 -3.259265
H -6.593275 -2.954378 -1.799096
H -6.431099 -1.273285 0.038860
H -4.312361 -0.048979 0.421768
C -2.067557 1.656636 -1.202116
C -2.986579 2.064596 -2.179681
C -3.233188 3.418309 -2.414566
C -2.554956 4.376525 -1.659435
C -1.635218 3.996848 -0.676390
C -1.389002 2.637987 -0.445605
O -0.487211 2.199320 0.510398
C 0.314327 3.184158 1.183541
H 1.041400 2.635394 1.786736
H 0.856382 3.803088 0.454248
H -0.310518 3.817134 1.832856
H -1.129285 4.768190 -0.098347
H -2.741165 5.440087 -1.827066
H -3.952284 3.721285 -3.178258
H -3.522110 1.306137 -2.756104
H -0.341145 -1.690141 -2.055344
H -0.844435 -0.364354 -3.134617
H 1.606953 -0.131713 -2.621835
H 0.705647 1.217838 -1.907449

^{4}5B-12
Geometry with 79 atoms:
Total energy: -3195.952807900
Cr -0.491603 -0.375994 1.261093
C -0.010629 -0.410582 3.247204
C -1.485475 -0.140926 3.377135
C -2.385131 -1.208068 4.014279
C -2.246292 -2.624216 3.436489
C -2.316214 -2.725820 1.902778
C -1.009359 -2.372031 1.182751
H -1.059863 -2.671790 0.120339
H -0.180089 -2.939296 1.639280
H -2.586719 -3.767708 1.646573
H -3.154802 -2.112762 1.519864
H -3.044723 -3.240702 3.881348
H -1.298071 -3.077082 3.775505
H -2.171677 -1.231443 5.096303
H -3.434461 -0.879262 3.911877
H -1.691724 0.849663 3.815707
H -1.971703 0.019086 2.329335
H 0.636653 0.385804 3.638271
H 0.321132 -1.392743 3.606293
P 1.522968 -0.270850 -0.227403
C 2.662930 1.043671 0.360776
C 3.209916 0.872743 1.644593
C 4.047981 1.846801 2.191232
C 4.341032 3.006611 1.465311
C 3.803931 3.179379 0.185854
C 2.973040 2.200682 -0.368869
H 2.580314 2.346137 -1.376177
H 4.038947 4.078105 -0.390072
H 4.991642 3.772497 1.894581
H 4.468761 1.702502 3.189372
H 2.971459 -0.023469 2.224438
C 2.600164 -1.705659 -0.572122
C 2.394670 -2.919440 0.098019
C 3.232771 -4.015610 -0.122650
C 4.293930 -3.893979 -1.020760
C 4.528466 -2.692265 -1.696850
C 3.687130 -1.592524 -1.478089
O 3.838593 -0.393214 -2.084653
C 4.968844 -0.142213 -2.905523
H 5.911103 -0.289027 -2.350625
H 4.895630 0.909136 -3.214081
H 4.968889 -0.781975 -3.804881
H 5.366332 -2.620724 -2.390207
H 4.957827 -4.742837 -1.202899
H 3.057248 -4.954247 0.406743
H 1.570282 -3.003703 0.805316
C 0.857228 0.297959 -1.879917
C -0.501472 -0.336574 -2.204865
P -1.716286 0.060631 -0.858543
C -3.321652 -0.651590 -1.338901
C -4.447873 -0.320119 -0.562178
C -5.687155 -0.897887 -0.836853
C -5.814262 -1.823009 -1.880164
C -4.699042 -2.161412 -2.649888
C -3.454856 -1.578735 -2.384744
H -2.597101 -1.857514 -2.999659
H -4.793538 -2.882717 -3.465263
H -6.784044 -2.280281 -2.090706
H -6.556862 -0.630108 -0.231915
H -4.355749 0.395889 0.259636
C -1.904725 1.878517 -0.942673
C -2.680957 2.508806 -1.926387
C -2.803324 3.898299 -1.963959
C -2.141334 4.666509 -1.004025
C -1.361885 4.063304 -0.012093
C -1.240465 2.668047 0.022402
O -0.482250 2.013369 0.977680
C 0.257710 2.810707 1.917545
H 0.841135 2.114016 2.524329
H 0.949464 3.485959 1.393366
H -0.427467 3.382447 2.562636
H -0.864152 4.690630 0.725008
H -2.230817 5.755392 -1.016384
H -3.413115 4.376546 -2.733150
H -3.204094 1.895294 -2.664544
H -0.420438 -1.434528 -2.259935
H -0.874461 0.023068 -3.177130
H 1.597844 0.078794 -2.659757
H 0.752641 1.392586 -1.829143

^{4}5B-13
Geometry with 79 atoms:
Total energy: -3195.953408880
Cr -0.008376 0.133680 1.055624
C -1.550398 0.307954 2.423130
C -1.731625 1.690700 3.064730
C -0.899129 1.953507 4.326195
C 0.630331 1.961056 4.190907
C 1.304759 0.609912 3.872000
C 1.570223 0.326914 2.389995
H 2.080964 -0.651159 2.292644
H 2.288155 1.073287 2.000651
H 2.272484 0.576426 4.409628
H 0.705480 -0.205659 4.315029
H 1.034508 2.334661 5.147244
H 0.931840 2.709057 3.434986
H -1.208936 2.929629 4.740666
H -1.176503 1.203986 5.091031
H -1.538270 2.494095 2.328343
H -2.794058 1.825639 3.345565
H -1.368944 -0.453116 3.203581
H -2.482114 0.011085 1.908578
P -1.562193 -0.240959 -0.932382
C -3.172692 -1.095969 -0.869580
C -3.309053 -2.419654 -1.326126
C -4.515896 -3.104050 -1.154757
C -5.596279 -2.480612 -0.523827
C -5.466837 -1.166052 -0.063577
C -4.264025 -0.476766 -0.230747
H -4.178638 0.550808 0.129476
H -6.307545 -0.671537 0.428977
H -6.538800 -3.017372 -0.392264
H -4.611339 -4.129176 -1.521129
H -2.479613 -2.928362 -1.821824
C -1.928876 1.504628 -1.336894
C -2.920752 1.868150 -2.262577
C -3.210943 3.207496 -2.520196
C -2.507338 4.202118 -1.836697
C -1.514097 3.869166 -0.912265
C -1.219546 2.523174 -0.664837
O -0.220548 2.157881 0.232505
C 0.777977 3.149058 0.555995
H 1.162206 3.606530 -0.367435
H 1.585636 2.622449 1.068852
H 0.359452 3.916122 1.222507
H -0.987374 4.663994 -0.386879
H -2.731601 5.256186 -2.016533
H -3.985704 3.473172 -3.242189
H -3.481820 1.082409 -2.774792
C -0.662791 -0.926267 -2.412233
C 0.730019 -0.297001 -2.530284
P 1.598696 -0.289172 -0.883105
C 3.207877 0.525922 -1.161183
C 4.192592 0.419356 -0.159133
C 5.404190 1.099551 -0.286750
C 5.648084 1.900501 -1.408260
C 4.674816 2.014122 -2.404201
C 3.459243 1.332011 -2.285237
H 2.719789 1.433659 -3.081725
H 4.861835 2.632435 -3.285616
H 6.597370 2.432622 -1.506120
H 6.161711 1.004166 0.495046
H 4.013306 -0.202477 0.720257
C 1.989771 -2.039610 -0.498531
C 3.059356 -2.719635 -1.102868
C 3.381986 -4.027007 -0.738537
C 2.637460 -4.664083 0.256707
C 1.568184 -4.011411 0.875956
C 1.237292 -2.707380 0.492532
O 0.162608 -2.038364 1.068892
C -0.880310 -2.824979 1.684763
H -1.091871 -3.711233 1.070049
H -0.585831 -3.121801 2.701952
H -1.773437 -2.195290 1.726799
H 1.011546 -4.521775 1.660632
H 2.889774 -5.681038 0.566052
H 4.216381 -4.540749 -1.220330
H 3.655711 -2.206271 -1.861274
H 0.636365 0.759550 -2.831050
H 1.336471 -0.810746 -3.292466
H -1.249319 -0.772860 -3.331483
H -0.573710 -2.012753 -2.250951

^{4}5B-14
Geometry with 79 atoms:
Total energy: -3195.954351160
Cr -0.031860 -0.729345 0.904145
C 1.659796 -1.157695 2.016860
C 2.141742 -2.613754 2.053052

C 1.468910 -3.523977 3.087759
C -0.032006 -3.806995 2.927747
C -0.989371 -2.634818 3.225442
C -1.414544 -1.788551 2.022706
H -2.123926 -1.004333 2.352664
H -1.988230 -2.422685 1.321547
H -1.901453 -3.047738 3.698678
H -0.531836 -1.999820 4.006526
H -0.278232 -4.637277 3.611274
H -0.230106 -4.195807 1.911304
H 1.999741 -4.492753 3.078123
H 1.639312 -3.103166 4.096787
H 2.052644 -3.085149 1.057520
H 3.227938 -2.628988 2.268528
H 1.481218 -0.799121 3.046044
H 2.459576 -0.510830 1.613922
P 1.364723 0.562017 -0.877717
C 2.712382 1.743244 -0.519682
C 2.493044 3.130278 -0.609447
C 3.482895 4.030626 -0.206923
C 4.699794 3.563034 0.297023
C 4.922484 2.186409 0.399629
C 3.937718 1.281015 -0.001264
H 4.131548 0.210106 0.083708
H 5.870108 1.811184 0.793597
H 5.472644 4.269177 0.609839
H 3.298738 5.104630 -0.289642
H 1.549684 3.526724 -0.989400
C 2.145468 -0.921236 -1.624139
C 3.305604 -0.874567 -2.413511
C 3.872098 -2.041728 -2.927895
C 3.279972 -3.276667 -2.651587
C 2.119613 -3.349705 -1.876876
C 1.554032 -2.174466 -1.375884
O 0.381442 -2.207864 -0.621478
C -0.581468 -3.233344 -0.947541
H -0.336464 -4.172378 -0.431718
H -0.600195 -3.388481 -2.035853
H -1.559481 -2.875980 -0.610252
H 1.671271 -4.318626 -1.658253
H 3.723627 -4.197692 -3.036482
H 4.775878 -1.987334 -3.538326
H 3.774516 0.090471 -2.618191
C 0.355586 1.296901 -2.264952
C -1.011188 0.607525 -2.378239
P -1.759904 0.326095 -0.689207
C -3.517753 -0.061181 -0.993308
C -4.497626 0.339480 -0.067779
C -5.829741 -0.040416 -0.245372
C -6.198258 -0.827227 -1.341539
C -5.227655 -1.235554 -2.261320
C -3.892772 -0.859117 -2.089588
H -3.150284 -1.191465 -2.818934
H -5.510077 -1.848898 -3.120619
H -7.241397 -1.121897 -1.478769
H -6.584173 0.282226 0.476291
H -4.221545 0.956469 0.790882
C -1.721040 2.004954 0.050612
C -2.261781 3.121421 -0.608045
C -2.128179 4.405202 -0.080365
C -1.435574 4.582637 1.121198
C -0.894535 3.489658 1.801254
C -1.046306 2.201936 1.272479
O -0.534606 1.092263 1.932494
C -0.376243 1.178470 3.366177
H -0.330573 0.153134 3.742180
H 0.554532 1.707201 3.616358
H -1.245066 1.689781 3.804449
H -0.352067 3.650560 2.732035
H -1.311353 5.583790 1.540574
H -2.557351 5.262252 -0.603454
H -2.796532 2.974566 -1.549956
H -0.913357 -0.383811 -2.850028
H -1.696581 1.198804 -3.005541
H 0.914075 1.238846 -3.211738
H 0.210312 2.360946 -2.029489

^{4}5B-15
Geometry with 79 atoms:
Total energy: -3195.953252820
Cr -0.480643 -1.154395 0.858184
C 0.172040 -2.211311 2.475442
C -1.312119 -2.357186 2.713996
C -1.925096 -3.759386 2.595354
C -1.563621 -4.537870 1.322792
C -1.784385 -3.783724 0.001602
C -0.668224 -2.803594 -0.382038
H -0.836828 -2.436772 -1.410273
H 0.303953 -3.327063 -0.391849
H -1.877532 -4.537127 -0.803949
H -2.764802 -3.269445 0.025683
H -2.166383 -5.461056 1.320749
H -0.512107 -4.871446 1.368199
H -1.611710 -4.340618 3.479091
H -3.023257 -3.664059 2.659281
H -1.642534 -1.876459 3.650029
H -1.922073 -1.721455 1.956189
H 0.714907 -1.649029 3.248432
H 0.691750 -3.152182 2.258644
P 1.409314 -0.281825 -0.440531
C 1.914987 1.377697 0.152475
C 1.760145 2.551434 -0.598682
C 2.130303 3.785901 -0.056859
C 2.663829 3.857845 1.232974
C 2.823707 2.689161 1.985987
C 2.444867 1.456089 1.451570
H 2.568037 0.545759 2.045303
H 3.245367 2.738325 2.993215
H 2.955128 4.823902 1.652369
H 2.000221 4.695599 -0.647768
H 1.356544 2.516384 -1.611438
C 2.957378 -1.237068 -0.572779
C 3.099248 -2.436004 0.140111
C 4.290588 -3.164171 0.091784
C 5.353817 -2.682741 -0.674065
C 5.240010 -1.487797 -1.391758
C 4.042232 -0.759670 -1.350961
O 3.838246 0.399401 -2.015990
C 4.907355 1.021359 -2.711483
H 5.262413 0.400458 -3.552102
H 5.752090 1.243278 -2.037128
H 4.508009 1.965244 -3.105975
H 6.084699 -1.132379 -1.981413
H 6.292846 -3.240270 -0.718409
H 4.386369 -4.096514 0.651824
H 2.265802 -2.792493 0.746337
C 0.765709 -0.100564 -2.174861
C -0.657591 0.483847 -2.300507
P -1.701962 0.315117 -0.749860
C -3.418598 0.059266 -1.326970
C -3.678779 -1.045165 -2.160973
C -4.984940 -1.335092 -2.558725
C -6.046806 -0.535809 -2.121087
C -5.796292 0.552092 -1.280535
C -4.489944 0.850385 -0.880517
H -4.311647 1.702351 -0.221714
H -6.622039 1.177603 -0.932435
H -7.068885 -0.763686 -2.432963
H -5.174421 -2.191664 -3.210134
H -2.861976 -1.688907 -2.498663
C -1.627885 1.971709 0.019159
C -1.985727 3.133948 -0.683065
C -1.864958 4.395106 -0.101733
C -1.375018 4.496558 1.202383
C -1.014696 3.357150 1.924463
C -1.141327 2.090495 1.338591
O -0.789102 0.932411 2.007126
C -0.460491 1.045825 3.399528
H 0.460154 1.631717 3.537404
H -1.293059 1.504913 3.954223
H -0.295310 0.031469 3.771361
H -0.622448 3.474266 2.932153
H -1.264021 5.476767 1.672057
H -2.148211 5.289603 -0.660231
H -2.369689 3.043378 -1.702497
H -1.196827 -0.016707 -3.117397
H -0.628296 1.552449 -2.557199
H 0.788693 -1.134603 -2.551594
H 1.490772 0.469789 -2.770728

^{4}5B-16
Geometry with 79 atoms:
Total energy: -3195.952365370
Cr 0.443825 1.246350 0.781867
C -0.211778 2.422801 2.316299
C 1.270210 2.591711 2.528789
C 1.873625 3.986634 2.317971
C 1.487785 4.682027 1.004626
C 1.696808 3.846631 -0.268539
C 0.602926 2.811847 -0.564888
H 0.776825 2.376747 -1.565074
H -0.383064 3.308148 -0.602052
H 1.752240 4.546614 -1.123789
H 2.691316 3.361151 -0.234323
H 2.083006 5.607512 0.935367
H 0.434614 5.010697 1.044949
H 1.568660 4.617959 3.169619
H 2.973494 3.902564 2.372085
H 1.617191 2.163450 3.483670
H 1.874957 1.919950 1.792779
H -0.752311 1.927913 3.135397
H -0.736059 3.338130 2.017093
P -1.437760 0.230396 -0.446428
C -1.900691 -1.401658 0.248535
C -2.456409 -1.412770 1.538941
C -2.796217 -2.620905 2.150783
C -2.571699 -3.830998 1.484590
C -2.013145 -3.825618 0.203598
C -1.681186 -2.617023 -0.415557
H -1.255074 -2.636231 -1.419386
H -1.832162 -4.767412 -0.319856
H -2.832458 -4.777250 1.964828
H -3.237718 -2.618310 3.150639
H -2.627110 -0.470050 2.066673
C -3.006602 1.138473 -0.642495
C -3.178956 2.377042 -0.008646
C -4.381092 3.080128 -0.121783
C -5.422913 2.533889 -0.873697
C -5.279244 1.297217 -1.511148
C -4.071806 0.592532 -1.402777
O -3.838766 -0.604698 -1.985396
C -4.882944 -1.286728 -2.661655
H -5.742373 -1.472269 -1.995064
H -4.463230 -2.250614 -2.978998
H -5.222252 -0.731064 -3.552892
H -6.107683 0.891812 -2.091924
H -6.368861 3.072799 -0.970264
H -4.501719 4.044181 0.376337
H -2.360557 2.784833 0.586093
C -0.790562 -0.041021 -2.166372
C 0.651636 -0.585660 -2.265460
P 1.695421 -0.291782 -0.737358
C 3.412350 -0.089270 -1.333732
C 4.285102 0.692934 -0.558178
C 5.617151 0.860045 -0.945130
C 6.087641 0.253539 -2.113646
C 5.223593 -0.520700 -2.894952
C 3.891729 -0.693371 -2.509657
H 3.233390 -1.302622 -3.133497
H 5.587779 -0.993908 -3.810112
H 7.128171 0.387833 -2.419023
H 6.286517 1.471949 -0.335721
H 3.921927 1.179916 0.350913
C 1.666609 -1.895782 0.153273
C 2.118386 -3.083502 -0.441206
C 2.066387 -4.299190 0.238986
C 1.559116 -4.327679 1.539833
C 1.114636 -3.158463 2.160239
C 1.167700 -1.938751 1.472105
O 0.736675 -0.754275 2.045508
C 0.391027 -0.785026 3.438316
H 0.146642 0.239262 3.730721
H -0.488050 -1.423739 3.608245
H 1.243649 -1.140297 4.037256
H 0.720629 -3.217072 3.172421
H 1.506829 -5.270829 2.088829
H 2.421383 -5.214097 -0.239716
H 2.525450 -3.051259 -1.454872
H 1.167279 -0.091538 -3.101703
H 0.655589 -1.664575 -2.478540
H -0.843983 0.967341 -2.604846
H -1.497899 -0.667486 -2.725371

^{4}5B-17
Geometry with 79 atoms:
Total energy: -3195.952244800
Cr -0.200279 -0.957635 0.600126
C -0.648608 -2.457242 -0.763518
C -1.072807 -3.780568 -0.118764
C -2.573943 -3.924396 0.162988
C -3.211686 -2.848376 1.055541
C -2.408113 -2.522293 2.329912
C -1.504357 -1.297618 2.180128
H -0.858004 -1.175409 3.076284
H -2.134498 -0.386098 2.154661
H -3.110438 -2.362458 3.170220
H -1.813493 -3.407260 2.624293
H -4.226632 -3.189631 1.320955
H -3.354572 -1.918576 0.480333
H -3.114126 -3.951168 -0.801299
H -2.738659 -4.912980 0.629006
H -0.777429 -4.622801 -0.774007
H -0.508400 -3.948618 0.816933
H 0.293919 -2.610617 -1.320429
H -1.401836 -2.148006 -1.511162
P -1.439254 0.638321 -0.694651
C -3.246570 0.524400 -0.916331
C -3.779610 -0.324274 -1.903677
C -5.157232 -0.540618 -1.976111
C -6.015167 0.076672 -1.060518
C -5.490347 0.913011 -0.070765
C -4.113404 1.135587 0.006352
H -3.716891 1.785628 0.789162
H -6.155729 1.395147 0.649445
H -7.092411 -0.097124 -1.116768
H -5.560412 -1.200048 -2.748359
H -3.125576 -0.835333 -2.614144
C -1.096881 2.237182 0.125987
C -1.613293 3.445812 -0.368736
C -1.325806 4.660243 0.252655
C -0.511820 4.668426 1.389073
C 0.014581 3.481880 1.903437
C -0.272419 2.263710 1.273391
O 0.234693 1.066846 1.720468
C 1.083723 1.048504 2.871310
H 0.530474 1.357584 3.771691
H 1.962015 1.693598 2.719989
H 1.421219 0.012312 2.991883
H 0.649547 3.518731 2.786856
H -0.279475 5.611455 1.889665
H -1.737031 5.591584 -0.141711
H -2.259723 3.426125 -1.250382
C -0.698547 0.810036 -2.418672
C 0.692881 0.146534 -2.578856
P 1.546552 0.003250 -0.940677
C 2.515504 1.521968 -0.658032
C 2.159693 2.739204 -1.263578
C 2.827693 3.918606 -0.922510
C 3.852937 3.898830 0.026789
C 4.215154 2.689909 0.631701
C 3.551280 1.508556 0.295269
H 3.847071 0.571091 0.773626
H 5.023962 2.665722 1.366424
H 4.373887 4.822136 0.291351
H 2.540881 4.857470 -1.402071
H 1.357574 2.783674 -2.001519
C 2.732930 -1.379306 -0.925571
C 3.713175 -1.568370 -1.909394
C 4.589658 -2.652706 -1.849731
C 4.487328 -3.553485 -0.788144
C 3.523576 -3.384010 0.211665
C 2.645364 -2.297542 0.148211
O 1.671214 -2.079049 1.120535
C 1.686136 -2.902147 2.302088
H 1.486635 -3.953737 2.050693
H 2.654167 -2.808836 2.817356
H 0.883118 -2.532039 2.948276
H 3.470851 -4.108700 1.022502
H 5.165507 -4.407965 -0.727645
H 5.346534 -2.792358 -2.624201
H 3.787238 -0.851380 -2.731351
H 1.305183 0.677224 -3.323371
H 0.576298 -0.891646 -2.922147
H -0.660076 1.887490 -2.636055
H -1.406726 0.376386 -3.137658

^{4}5B-18
Geometry with 79 atoms:
Total energy: -3195.950951480
Cr -0.135998 -0.961338 0.569552
C -0.440526 -2.493342 -0.794006
C -0.073601 -3.908534 -0.324752
C -0.492369 -4.308400 1.097875
C -1.969738 -4.149974 1.479872
C -2.537235 -2.712221 1.504051
C -1.548137 -1.625657 1.936507
H -0.989399 -1.934097 2.847165
H -2.095993 -0.706231 2.218871
H -2.942510 -2.452482 0.511920
H -3.420864 -2.718315 2.170828
H -2.084361 -4.583070 2.489959
H -2.592988 -4.776564 0.816656
H -0.210098 -5.365502 1.250219
H 0.108632 -3.742641 1.825583
H -0.508579 -4.642857 -1.031916
H 1.020243 -4.046389 -0.404609
H 0.098895 -2.285343 -1.736002
H -1.516128 -2.450486 -1.034522
P -1.580623 0.480458 -0.696431
C -3.359631 0.133120 -0.901442
C -4.296446 0.657192 0.005996
C -5.636926 0.271257 -0.068315
C -6.054551 -0.642606 -1.040464
C -5.125342 -1.174980 -1.939671
C -3.783029 -0.796072 -1.869260
H -3.069552 -1.238621 -2.568350
H -5.444778 -1.893951 -2.697792
H -7.103636 -0.942967 -1.095546
H -6.357790 0.686889 0.639911
H -3.982583 1.365938 0.774737
C -1.447891 2.097439 0.148060
C -2.080783 3.244136 -0.358117
C -1.933865 4.482385 0.265480
C -1.141842 4.577061 1.413353
C -0.503744 3.452385 1.940202
C -0.655136 2.209273 1.311123
O -0.043558 1.067790 1.774489
C 0.809149 1.152389 2.918973
H 1.186772 0.140840 3.101373
H 0.247074 1.486247 3.804989
H 1.658698 1.825923 2.725607
H 0.111326 3.560529 2.831959
H -1.013554 5.540489 1.912464
H -2.433948 5.365156 -0.137920
H -2.703489 3.158656 -1.252619
C -0.889218 0.789591 -2.420765
C 0.597239 0.382631 -2.593577
P 1.460055 0.254494 -0.955297
C 2.263949 1.857299 -0.619118
C 3.389183 1.918981 0.222968
C 3.924580 3.155227 0.592555
C 3.342887 4.341632 0.132038
C 2.224040 4.286455 -0.704172
C 1.684039 3.053257 -1.077566
H 0.798871 3.035899 -1.715834
H 1.762522 5.207849 -1.066936
H 3.764675 5.307184 0.421201
H 4.805113 3.191417 1.238965
H 3.857114 0.999341 0.583432
C 2.778143 -0.999730 -1.015582
C 3.702039 -1.120419 -2.063311
C 4.679516 -2.116734 -2.043669
C 4.740428 -2.994890 -0.959436
C 3.835427 -2.891044 0.101680
C 2.852072 -1.898140 0.073736
O 1.920642 -1.758582 1.101181
C 2.236133 -2.336452 2.379804
H 2.274537 -3.432934 2.325706
H 3.196362 -1.940725 2.745534
H 1.425806 -2.050670 3.060673
H 3.899868 -3.594576 0.930502
H 5.500770 -3.779027 -0.931694
H 5.391473 -2.204526 -2.866859
H 3.654893 -0.420461 -2.901515
H 1.121607 1.073025 -3.270632
H 0.662220 -0.623602 -3.031602
H -1.038965 1.858991 -2.631135
H -1.515330 0.240711 -3.137777

^{4}5B-19
Geometry with 79 atoms:
Total energy: -3195.950826100
Cr -0.006976 -0.098431 1.088732
C -1.685318 -0.189357 2.314167
C -1.580309 0.148960 3.804500
C -0.802035 -0.828812 4.698689
C 0.723910 -0.666822 4.776035
C 1.567508 -1.154800 3.590330
C 1.637525 -0.252572 2.354021
H 2.426309 -0.652183 1.688855
H 1.999422 0.751364 2.643310
H 2.600036 -1.298299 3.965868
H 1.234641 -2.171257 3.311523
H 1.062818 -1.219554 5.669582
H 0.964426 0.394090 4.981359
H -1.187998 -0.715976 5.726420
H -1.046638 -1.868950 4.410373
H -1.158849 1.161126 3.942305
H -2.608945 0.220120 4.209970
H -2.190532 -1.164420 2.182830
H -2.365919 0.546228 1.844088
P -1.539458 0.159145 -0.930396
C -3.195559 -0.582073 -1.112513
C -3.330561 -1.835747 -1.737932
C -4.573033 -2.472872 -1.777270
C -5.689761 -1.874889 -1.184243
C -5.559379 -0.635493 -0.550742
C -4.320525 0.009342 -0.510814
H -4.233985 0.978265 -0.014980
H -6.427544 -0.163869 -0.083934
H -6.660473 -2.375408 -1.215580
H -4.668588 -3.441483 -2.274197
H -2.468498 -2.325286 -2.197969
C -1.766747 1.974527 -0.847934
C -2.561932 2.644627 -1.793211
C -2.676123 4.033552 -1.792116
C -1.973533 4.770596 -0.836426
C -1.176177 4.132083 0.115843
C -1.074701 2.733177 0.120244
O -0.293123 2.071035 1.059276
C 0.214860 2.846308 2.166258
H 1.002240 3.531158 1.818251
H 0.638842 2.136927 2.878363
H -0.602582 3.402019 2.646686
H -0.640923 4.738037 0.843885
H -2.042283 5.860865 -0.822902
H -3.303565 4.535746 -2.531187
H -3.105911 2.057882 -2.537972
C -0.675493 -0.035484 -2.573321
C 0.717998 0.600436 -2.494795
P 1.554579 0.071774 -0.914710
C 3.207465 0.842329 -0.922476
C 4.334074 0.147104 -0.448421
C 5.569992 0.792306 -0.355265
C 5.695270 2.133952 -0.727868
C 4.576482 2.833745 -1.191339
C 3.337156 2.196078 -1.283883
H 2.473932 2.763914 -1.639546
H 4.667906 3.882717 -1.483870
H 6.663715 2.634768 -0.656376
H 6.439963 0.240762 0.009453
H 4.251333 -0.902046 -0.156798
C 1.800138 -1.720822 -1.196817
C 2.629878 -2.178578 -2.234139
C 2.764055 -3.537948 -2.510482
C 2.048634 -4.458628 -1.742338
C 1.217012 -4.033137 -0.703896
C 1.095031 -2.665131 -0.419764
O 0.279082 -2.210413 0.609880
C -0.402118 -3.201485 1.408698
H -1.162177 -3.715944 0.801386
H 0.317626 -3.921042 1.821872
H -0.886312 -2.668015 2.227701
H 0.675812 -4.780657 -0.128357
H 2.133308 -5.528687 -1.946140
H 3.416287 -3.875024 -3.318573

H	3.184266	-1.447683	-2.828230
H	0.638859	1.698730	-2.475673
H	1.334831	0.323623	-3.363628
H	-1.278887	0.417658	-3.374949
H	-0.595113	-1.113469	-2.784114

^{45}C-01
Geometry with 83 atoms:
Total energy: -3124.209554810

Cr	0.031902	-0.680024	1.183702
P	-1.762194	0.085013	-0.311839
C	-3.154347	-1.063154	-0.568595
C	-3.523366	-1.560291	-1.828244
C	-4.588854	-2.458347	-1.940352
C	-5.290210	-2.864505	-0.801512
C	-4.918700	-2.379524	0.457540
C	-3.851058	-1.488596	0.576459
H	-3.555807	-1.121552	1.562849
H	-5.460342	-2.699608	1.350849
H	-6.124832	-3.563619	-0.893868
H	-4.872887	-2.839226	-2.924290
H	-2.995941	-1.247075	-2.731430
C	-2.386923	1.732829	0.213077
C	-3.426426	2.465024	-0.411170
C	-3.719836	3.744113	0.093489
C	-3.022428	4.297704	1.167622
C	-1.996952	3.572950	1.780000
C	-1.691835	2.301048	1.300121
H	-0.892598	1.730608	1.784990
H	-1.441972	3.992325	2.622052
H	-3.279294	5.297511	1.526190
H	-4.519542	4.320829	-0.379776
C	-4.271581	1.941592	-1.553880
C	-5.634175	1.406696	-1.090771
H	-6.220738	1.044953	-1.949894
H	-5.514505	0.570511	-0.386040
H	-6.217787	2.193364	-0.586782
H	-3.747540	1.149775	-2.103257
H	-4.430364	2.761687	-2.273724
C	-0.938441	0.365149	-1.955728
C	0.312426	1.239118	-1.777441
P	1.532141	0.531544	-0.555286
C	2.592778	1.966405	-0.142935
C	2.579949	2.479468	1.163196
C	3.383229	3.572865	1.500148
C	4.203783	4.159376	0.532446
C	4.220772	3.653072	-0.772687
C	3.421089	2.559603	-1.110938
H	3.455970	2.154886	-2.125755
H	4.866328	4.107990	-1.527892
H	4.835785	5.011011	0.795839
H	3.372558	3.962812	2.520786
H	1.950779	2.017825	1.929913
C	2.600176	-0.636446	-1.492966
C	2.321251	-0.945377	-2.836972
C	3.066004	-1.904686	-3.524718
C	4.101583	-2.573644	-2.869090
C	4.383392	-2.273333	-1.536035
C	3.650453	-1.312351	-0.822024
C	4.046994	-1.026520	0.612528
C	5.295014	-0.141286	0.733998
H	6.162542	-0.619619	0.252408
H	5.548207	0.032518	1.792045
H	5.141854	0.836765	0.255152
H	4.234797	-1.985657	1.123537
H	3.212809	-0.555297	1.156820
H	5.193476	-2.801810	-1.025327
H	4.687943	-3.331863	-3.393787
H	2.833805	-2.128409	-4.568595
H	1.513432	-0.439816	-3.367493
H	0.797939	1.443148	-2.743904
H	0.035357	2.219927	-1.357900
H	-0.681165	-0.630423	-2.351654
H	-1.632081	0.837493	-2.667055
C	-0.889135	-1.282514	2.883362
C	0.528278	-1.537145	3.331598
C	0.978979	-2.995246	3.503706
C	0.621656	-3.958221	2.361512
H	-0.466156	-4.144973	2.349065
H	1.085917	-4.929747	2.597821
C	1.063760	-3.514834	0.957681
C	0.140393	-2.507939	0.272880
H	-0.896481	-2.885080	0.235752
H	0.477184	-2.310314	-0.759684
H	1.118831	-4.414546	0.315233
H	2.099732	-3.131027	0.993426
H	0.533931	-3.370290	4.440896
H	2.072528	-3.005168	3.655925
H	0.807817	-0.947187	4.220578
H	1.279783	-1.075026	2.570842
H	-1.532158	-2.167734	2.810596
H	-1.398131	-0.466950	3.420724

^{45}C-02
Geometry with 83 atoms:
Total energy: -3124.212056970

Cr	-0.194041	-0.581636	1.117732
P	-1.900762	0.048391	-0.521714
C	-3.255382	-1.149768	-0.757816
C	-4.036192	-1.464535	0.369005
C	-5.073400	-2.391824	0.266932
C	-5.333513	-3.021246	-0.956237
C	-4.556806	-2.716607	-2.076829
C	-3.519774	-1.782365	-1.982690
H	-2.927541	-1.556899	-2.871519
H	-4.756991	-3.206621	-3.032824
H	-6.142223	-3.752017	-1.033848
H	-5.677042	-2.630375	1.145921
H	-3.826118	-0.985315	1.329386
C	-2.702333	1.709779	-0.458951
C	-2.310915	2.731937	0.435348
C	-2.928295	3.991422	0.310989
C	-3.910105	4.237904	-0.645225
C	-4.309014	3.215120	-1.512549
C	-3.704424	1.965008	-1.417908
H	-4.020247	1.169781	-2.097736
H	-5.085795	3.391879	-2.260086
H	-4.367929	5.227759	-0.713412
H	-2.626842	4.794213	0.989379
C	-1.311716	2.559323	1.561197
C	-1.965845	2.547147	2.946363
H	-2.464848	3.506657	3.152344
H	-2.727911	1.756115	3.018775
H	-1.216969	2.381800	3.737378
H	-0.560416	3.364275	1.509184
H	-0.738161	1.625475	1.420597
C	-0.953821	0.120854	-2.123684
C	0.287963	1.009209	-1.961172
P	1.438392	0.404698	-0.621751
C	2.483733	1.870485	-0.280523
C	2.449412	2.465929	0.989987
C	3.241473	3.584125	1.267723
C	4.072561	4.113652	0.276462
C	4.112799	3.523825	-0.992602
C	3.324831	2.405142	-1.271245
H	3.379349	1.935508	-2.256934
H	4.767412	3.933277	-1.765803
H	4.695084	4.984995	0.493911
H	3.213770	4.037601	2.261476
H	1.811596	2.051385	1.775226
C	2.551203	-0.832684	-1.401161
C	2.339463	-1.258326	-2.725437
C	3.136767	-2.250652	-3.297612
C	4.157543	-2.835245	-2.544953
C	4.369278	-2.422241	-1.229288
C	3.581154	-1.427249	-0.629749
C	3.898798	-1.022607	0.796274
C	5.131926	-0.116553	0.915810
H	4.996319	0.823854	0.362122
H	6.026865	-0.617452	0.514173
H	5.329804	0.134252	1.970202
H	4.065715	-1.936924	1.390057
H	3.033069	-0.521100	1.257509
H	5.166039	-2.885511	-0.640592
H	4.786163	-3.615581	-2.980685
H	2.958005	-2.564598	-4.328692
H	1.547652	-0.817866	-3.332912
H	0.824170	1.128633	-2.914828
H	-0.007656	2.022748	-1.643029
H	-0.677997	-0.912238	-2.387302
H	-1.605415	0.512529	-2.920301
C	-1.121967	-1.086660	2.841934
C	0.295686	-1.298637	3.307223
C	0.754399	-2.735273	3.594929
C	0.400053	-3.779715	2.526814
H	-0.686510	-3.973795	2.532400
H	0.872382	-4.729095	2.828190
C	0.834297	-3.431880	1.093968
C	-0.097243	-2.479472	0.341832
H	-1.132907	-2.860746	0.347634
H	0.226264	-2.374853	-0.708780
H	0.891150	-4.374081	0.515947
H	1.869268	-3.043859	1.099737
H	0.310584	-3.038903	4.558087
H	1.848056	-2.728220	3.746727
H	0.574214	-0.634431	4.142371
H	1.046857	-0.904886	2.507377
H	-1.750712	-1.984620	2.811848
H	-1.642594	-0.253767	3.334789

^{45}C-03
Geometry with 83 atoms:
Total energy: -3124.211024060

Cr	-0.218102	-0.442897	1.198052
P	-1.903794	0.118981	-0.498485
C	-3.166842	-1.178780	-0.737104
C	-3.397537	-1.818794	-1.964467
C	-4.371563	-2.818981	-2.059849
C	-5.120274	-3.182231	-0.937943
C	-4.894885	-2.544747	0.287855
C	-3.920529	-1.551919	0.390739
H	-3.741077	-1.065224	1.352984
H	-5.476837	-2.826838	1.168629
H	-5.879800	-3.963933	-1.016446
H	-4.545191	-3.313388	-3.018734
H	-2.831532	-1.546654	-2.856976
C	-2.863965	1.693707	-0.397360
C	-2.483928	2.794274	0.405621
C	-3.327404	3.921741	0.420775
C	-4.493286	3.981788	-0.338168
C	-4.853361	2.897653	-1.144498
C	-4.046354	1.763924	-1.163976
H	-4.348022	0.910468	-1.774979
H	-5.765022	2.929479	-1.745538
H	-5.124076	4.873251	-0.298273
H	-3.057037	4.773727	1.050017
C	-1.220781	2.864158	1.243088
C	-0.253259	3.973232	0.815856
H	0.085985	3.840948	-0.223460
H	-0.729567	4.962954	0.882108
H	0.638202	3.989124	1.459985
H	-0.690833	1.896183	1.215134
H	-1.501341	3.011410	2.299861
C	-0.954397	0.243191	-2.094762
C	0.330554	1.065176	-1.910427
P	1.468575	0.352057	-0.613556
C	2.661781	1.705651	-0.296036
C	2.810157	2.205768	1.006156
C	3.728412	3.225943	1.270915
C	4.502101	3.754119	0.233593
C	4.360951	3.258570	-1.068217
C	3.448810	2.235278	-1.333065
H	3.362046	1.836084	-2.346985
H	4.970630	3.665733	-1.878448
H	5.221354	4.550556	0.439349
H	3.841478	3.606645	2.288820
H	2.214808	1.791353	1.824266
C	2.435656	-0.974953	-1.445573
C	2.167003	-1.336514	-2.778751
C	2.842138	-2.394500	-3.389148
C	3.798535	-3.110606	-2.666723
C	4.073782	-2.756021	-1.345879
C	3.410629	-1.694839	-0.709451
C	3.815169	-1.345420	0.708202
C	5.128136	-0.553153	0.781281
H	5.959456	-1.135124	0.353053
H	5.383553	-0.316015	1.826407
H	5.059374	0.392485	0.224271
H	3.926066	-2.279301	1.283484
H	3.016298	-0.776843	1.210298
H	4.826019	-3.317077	-0.784081
H	4.330075	-3.944919	-3.130803
H	2.618434	-2.656325	-4.426007

H 1.425696 -0.792376 -3.364733
H 0.855253 1.198156 -2.868649
H 0.091833 2.077996 -1.548729
H -0.723156 -0.787764 -2.405140
H -1.594695 0.693085 -2.869637
C -1.232605 -0.603168 2.939814
C 0.145405 -0.868073 3.492821
C 0.450236 -2.284285 4.001526
C 0.067265 -3.433107 3.056077
H -1.030827 -3.534951 3.007317
H 0.431576 -4.367612 3.513347
C 0.618194 -3.319221 1.624727
C -0.190876 -2.420736 0.688567
H -1.246646 -2.739114 0.659783
H 0.212191 -2.459630 -0.339231
H 0.640182 -4.334296 1.184186
H 1.676319 -3.001189 1.656156
H -0.075746 -2.414912 4.962368
H 1.529044 -2.347931 4.227828
H 0.460093 -0.117203 4.236618
H 0.957167 -0.671760 2.680299
H -1.942160 -1.434422 3.031003
H -1.685217 0.344353 3.269345

^{4}5C-04
Geometry with 83 atoms:
Total energy: -3124.211055560
Cr -0.117950 -0.612578 1.077139
P -1.888067 -0.026590 -0.514419
C -3.171213 -1.296134 -0.782765
C -3.458482 -1.850692 -2.040101
C -4.451077 -2.829033 -2.161909
C -5.161619 -3.255216 -1.036900
C -4.876513 -2.706627 0.218933
C -3.882218 -1.736587 0.348262
H -3.650369 -1.322833 1.333373
H -5.426696 -3.040954 1.101809
H -5.936903 -4.018832 -1.136718
H -4.669096 -3.257677 -3.143103
H -2.919055 -1.529891 -2.933276
C -2.799296 1.574168 -0.372565
C -2.497729 2.561770 0.591352
C -3.201596 3.780034 0.535129
C -4.181661 4.017918 -0.425049
C -4.490337 3.027872 -1.364325
C -3.800591 1.819293 -1.334916
H -4.049041 1.048265 -2.068615
H -5.264419 3.197573 -2.116297
H -4.708970 4.974878 -0.440302
H -2.970238 4.556158 1.269735
C -1.505739 2.382379 1.721159
C -2.175342 2.210438 3.087935
H -1.426645 2.044135 3.878771
H -2.753350 3.108030 3.357034
H -2.871994 1.358283 3.083960
H -0.819777 3.244640 1.744846
H -0.861992 1.507400 1.517531
C -0.976431 0.170797 -2.124783
C 0.197714 1.147041 -1.956068
P 1.409535 0.603828 -0.646766
C 2.350519 2.131467 -0.276543
C 2.195840 2.751167 0.973540
C 2.893756 3.925445 1.270632
C 3.754899 4.484007 0.321415
C 3.918921 3.867272 -0.924390
C 3.221904 2.694747 -1.224202
H 3.366652 2.209282 -2.192873
H 4.597470 4.299264 -1.664031
H 4.305157 5.398961 0.554370
H 2.770264 4.400383 2.246981
H 1.535201 2.311608 1.725207
C 2.594058 -0.531462 -1.477540
C 2.367474 -0.962167 -2.795925
C 3.204758 -1.902437 -3.400560
C 4.280439 -2.423715 -2.683215
C 4.514297 -2.001192 -1.371976
C 3.690751 -1.057471 -0.741325
C 3.976115 -0.598160 0.676614
C 4.908396 -1.476162 1.508522
H 4.971971 -1.090556 2.537978
H 5.932790 -1.490809 1.105193
H 4.550780 -2.517230 1.559031
H 3.015616 -0.497406 1.211720
H 4.380002 0.428820 0.636936
H 5.360909 -2.422632 -0.829041
H 4.942313 -3.162921 -3.141002
H 3.011942 -2.223245 -4.426929
H 1.530502 -0.570315 -3.375193
H 0.712384 1.323780 -2.912702
H -0.168327 2.129252 -1.615251
H -0.630618 -0.831162 -2.423590
H -1.667689 0.535241 -2.900507
C -1.005370 -1.296223 2.769929
C 0.423122 -1.389994 3.240421
C 1.028608 -2.785193 3.451156
C 0.796188 -3.798824 2.321050
H -0.261551 -4.113765 2.305660
H 1.370598 -4.705320 2.573433
C 1.192066 -3.325121 0.913304
C 0.159568 -2.444255 0.207494
H -0.830626 -2.931520 0.194253
H 0.462302 -2.252022 -0.836244
H 1.359297 -4.220766 0.285283
H 2.175314 -2.820928 0.949330
H 0.614209 -3.190231 4.389813
H 2.114311 -2.670778 3.616931
H 0.627338 -0.748774 4.114037
H 1.133824 -0.876758 2.473893
H -1.538996 -2.250103 2.681903
H -1.611083 -0.550129 3.302379

^{4}5C-05
Geometry with 83 atoms:
Total energy: -3124.209748240
Cr -0.154901 -0.370720 1.122028
P -1.920889 -0.075793 -0.573774
C -2.638306 -1.658601 -1.132073
C -3.237080 -2.472827 -0.152046
C -3.778187 -3.710468 -0.499843
C -3.710552 -4.158172 -1.824556
C -3.106651 -3.360396 -2.799273
C -2.573650 -2.112347 -2.458574
H -2.112341 -1.505392 -3.239671
H -3.050844 -3.706661 -3.834102
H -4.127513 -5.131193 -2.095194
H -4.247465 -4.331875 0.266580
H -3.280964 -2.133677 0.886244
C -3.327490 1.049047 -0.202218
C -3.098783 2.276288 0.467697
C -4.202163 3.109893 0.712230
C -5.492133 2.751453 0.318831
C -5.708522 1.538964 -0.340014
C -4.629288 0.695083 -0.600659
H -4.804249 -0.250199 -1.117471
H -6.714113 1.249499 -0.653940
H -6.329271 3.422505 0.526089
H -4.046805 4.065002 1.219329
C -1.717698 2.737577 0.895307
C -1.599213 3.187954 2.353349
H -0.557419 3.455310 2.594042
H -2.214440 4.076886 2.556699
H -1.922005 2.395675 3.046183
H -1.387754 3.555922 0.231418
H -0.983235 1.932144 0.710436
C -1.085292 0.708557 -2.041290
C 0.310701 0.122886 -2.287913
P 1.406426 0.368412 -0.798271
C 1.946586 2.120605 -0.926382
C 1.717857 3.002268 0.141880
C 2.124300 4.337646 0.059520
C 2.767257 4.800793 -1.091662
C 3.011390 3.925277 -2.156634
C 2.607402 2.591435 -2.074553
H 2.820103 1.911088 -2.903695
H 3.525314 4.282691 -3.052301
H 3.087083 5.843576 -1.157609
H 1.941507 5.014616 0.897679
H 1.229538 2.648379 1.052928
C 2.920317 -0.621586 -1.122555
C 3.055730 -1.370775 -2.304349
C 4.183501 -2.163230 -2.528025
C 5.188735 -2.214672 -1.563140
C 5.063484 -1.473143 -0.385761
C 3.944727 -0.664394 -0.138038
C 3.846320 0.157494 1.133056
C 4.710936 -0.292607 2.309280
H 4.479064 0.308574 3.202411
H 5.785796 -0.167862 2.106755
H 4.535825 -1.351660 2.558352
H 2.791749 0.169750 1.457307
H 4.074720 1.210391 0.888438
H 5.861700 -1.527472 0.355666
H 6.075296 -2.833083 -1.723213
H 4.270096 -2.737190 -3.453562
H 2.282239 -1.347866 -3.072603
H 0.239431 -0.961467 -2.463582
H 0.771006 0.575985 -3.179515
H -1.726608 0.615764 -2.931411
H -1.028268 1.785543 -1.816466
C -1.115596 -0.683124 2.882315
C 0.284684 -0.586611 3.432674
C 0.937168 -1.852288 4.004271
C 0.851895 -3.107117 3.123349
H -0.183472 -3.489518 3.108941
H 1.450885 -3.891873 3.613731
C 1.333297 -2.934234 1.672650
C 0.304123 -2.326770 0.718177
H -0.654685 -2.868883 0.774029
H 0.658713 -2.381266 -0.326086
H 1.607066 -3.933259 1.283066
H 2.278270 -2.358055 1.652342
H 0.465724 -2.061326 4.979385
H 1.998094 -1.629718 4.214212
H 0.407367 0.257403 4.131783
H 1.020721 -0.238079 2.599658
H -1.601702 -1.660201 2.997390
H -1.788435 0.129932 3.191147

^{4}5C-06
Geometry with 83 atoms:
Total energy: -3124.207618780
Cr 0.031910 -0.672847 1.001275
P 1.694055 0.208908 -0.630807
C 2.372309 1.911503 -0.576882
C 1.891321 2.853622 0.343958
C 2.395636 4.158736 0.337955
C 3.378904 4.527311 -0.583589
C 3.861142 3.589667 -1.504973
C 3.362041 2.286445 -1.503322
H 3.754686 1.554683 -2.214259
H 4.633301 3.873824 -2.223953
H 3.774065 5.546062 -0.584033
H 2.019216 4.886892 1.060417
H 1.131335 2.574800 1.073909
C 3.120592 -0.901899 -0.932092
C 4.079804 -1.084372 0.095020
C 5.126570 -1.990796 -0.133629
C 5.235460 -2.701942 -1.329528
C 4.285365 -2.517040 -2.336525
C 3.233700 -1.621577 -2.135886
H 2.501929 -1.491207 -2.934104
H 4.359644 -3.066766 -3.277733
H 6.060909 -3.403359 -1.473700
H 5.871507 -2.141831 0.652804
C 4.048146 -0.325122 1.406114
C 5.085662 0.803374 1.478871
H 6.107936 0.409424 1.363730
H 4.922557 1.548995 0.686840
H 5.029400 1.320540 2.449883
H 4.230742 -1.038750 2.226864
H 3.044425 0.087581 1.589774
C 0.693296 0.243793 -2.207955
C -0.588951 1.065852 -2.007390
P -1.664284 0.287227 -0.697203
C -2.389518 -1.160005 -1.567437
C -1.889022 -2.437627 -1.264375
C -2.396142 -3.571235 -1.905683
C -3.415560 -3.433443 -2.852211
C -3.922547 -2.164322 -3.157683
C -3.413296 -1.030647 -2.520274
H -3.826183 -0.044913 -2.749629
H -4.724156 -2.059414 -3.892960
H -3.820652 -4.317493 -3.350523

H	-2.001036	-4.560065	-1.660833
H	-1.102549	-2.556128	-0.508132
C	-3.040829	1.457812	-0.393864
C	-3.156249	2.643324	-1.145192
C	-4.179577	3.556711	-0.889695
C	-5.100570	3.296111	0.127730
C	-4.991771	2.124275	0.876826
C	-3.974511	1.186618	0.638487
C	-3.951570	-0.083347	1.461805
C	-4.958264	-1.140340	0.986739
H	-5.988279	-0.753288	1.037099
H	-4.904975	-2.041143	1.619187
H	-4.764014	-1.441415	-0.053385
H	-4.162046	0.172185	2.513304
H	-2.938750	-0.514810	1.453145
H	-5.713253	1.924734	1.674306
H	-5.903302	4.006683	0.339314
H	-4.254110	4.469679	-1.485112
H	-2.449708	2.868483	-1.945028
H	-0.341748	2.086381	-1.672471
H	-1.142627	1.146657	-2.955526
H	1.304225	0.671885	-3.017756
H	0.447682	-0.793632	-2.487009
C	1.003643	-2.212558	1.868143
C	-0.363247	-2.526747	2.417951
C	-0.580936	-2.353442	3.926893
C	-0.145159	-1.001993	4.511324
H	0.955424	-0.916717	4.497742
H	-0.431121	-0.994675	5.575699
C	-0.749518	0.227555	3.813104
C	-0.033875	0.664464	2.536034
H	1.022974	0.912044	2.741330
H	-0.526198	1.545636	2.084496
H	-0.724756	1.075462	4.524211
H	-1.822911	0.051958	3.614236
H	-0.036159	-3.164818	4.438393
H	-1.651365	-2.510862	4.146532
H	-0.745837	-3.505598	2.083608
H	-1.161466	-1.842614	1.922734
H	1.775147	-1.970642	2.609224
H	1.382839	-2.930470	1.124301

^{4}5C-07
Geometry with 83 atoms:
Total energy: -3124.210404520

Cr	-0.126962	-1.105693	0.826709
P	-1.927970	-0.090089	-0.522727
C	-3.504032	-0.974618	-0.804106
C	-3.647036	-2.284545	-0.318496
C	-4.830355	-2.992021	-0.549472
C	-5.875776	-2.394772	-1.259133
C	-5.741304	-1.085412	-1.735855
C	-4.561925	-0.373789	-1.508635
H	-4.473105	0.653258	-1.870655
H	-6.561501	-0.614645	-2.283219
H	-6.801580	-2.947396	-1.437140
H	-4.935783	-4.010781	-0.168807
H	-2.836054	-2.744902	0.248053
C	-2.373931	1.650065	-0.100661
C	-2.618383	2.025135	1.243056
C	-2.922961	3.368693	1.516501
C	-2.996433	4.326377	0.504749
C	-2.775092	3.949164	-0.821289
C	-2.470768	2.620371	-1.116941
H	-2.310335	2.349331	-2.161210
H	-2.840799	4.684431	-1.626507
H	-3.235075	5.363976	0.750460
H	-3.112240	3.664365	2.552232
C	-2.513080	1.059804	2.405729
C	-1.112725	1.043968	3.031855
H	-0.334100	0.763501	2.293971
H	-0.826872	2.043331	3.395035
H	-1.052937	0.340693	3.875247
H	-2.799360	0.042639	2.097100
H	-3.239727	1.355680	3.178573
C	-1.113365	0.013188	-2.193513
C	0.205346	0.802706	-2.159754
P	1.289892	0.483196	-0.656636
C	1.870256	2.185756	-0.277324
C	1.071098	3.007136	0.536351
C	1.440585	4.332007	0.780478
C	2.612848	4.847587	0.218563
C	3.410991	4.035796	-0.593863
C	3.042958	2.710673	-0.844737
H	3.673827	2.086051	-1.480755
H	4.325828	4.435495	-1.038276
H	2.903717	5.883040	0.411744
H	0.807702	4.961354	1.410890
H	0.147106	2.622941	0.971036
C	2.788278	-0.446006	-1.183150
C	2.908706	-0.955904	-2.487792
C	3.994974	-1.751225	-2.854403
C	4.980251	-2.049355	-1.910964
C	4.865188	-1.552762	-0.612645
C	3.780082	-0.754001	-0.217087
C	3.734579	-0.280175	1.224803
C	4.836710	0.723960	1.586971
H	5.837787	0.300302	1.411255
H	4.772022	1.003589	2.650548
H	4.748974	1.642930	0.989222
H	3.824208	-1.164378	1.879907
H	2.758049	0.168829	1.459222
H	5.632793	-1.799502	0.125999
H	5.834381	-2.673995	-2.183373
H	4.066990	-2.137142	-3.873803
H	2.146346	-0.743385	-3.238376
H	0.770506	0.655162	-3.091328
H	-0.004558	1.879624	-2.101978
H	-0.957260	-1.034012	-2.491827
H	-1.804686	0.445293	-2.933546
C	-0.874344	-2.325492	2.271461
C	0.583183	-2.430681	2.641599
C	1.270180	-3.793065	2.480783
C	1.048012	-4.487208	1.130736
H	0.011536	-4.860722	1.061491
H	1.687201	-5.385183	1.112253
C	1.351285	-3.624886	-0.103128
C	0.253335	-2.637806	-0.506765
H	-0.710241	-3.160009	-0.641690
H	0.516876	-2.176086	-1.471980
H	1.523132	-4.304332	-0.959446
H	2.311959	-3.095792	0.032795
H	0.911869	-4.447439	3.293227
H	2.353838	-3.659349	2.645546
H	0.802343	-2.002886	3.633903
H	1.224879	-1.715142	1.984096
H	-1.339301	-3.262060	1.940649
H	-1.504103	-1.818636	3.015353

^{4}5C-08
Geometry with 83 atoms:
Total energy: -3124.210712500

Cr	-0.187314	-0.871637	1.042084
P	-1.969352	0.021686	-0.471363
C	-3.447411	-0.997112	-0.828724
C	-3.699013	-2.138437	-0.050304
C	-4.824514	-2.927929	-0.305740
C	-5.702077	-2.583559	-1.336953
C	-5.458750	-1.443433	-2.112330
C	-4.339381	-0.649529	-1.858933
H	-4.172269	0.249182	-2.457451
H	-6.148016	-1.168676	-2.914414
H	-6.581493	-3.200864	-1.536272
H	-5.014943	-3.814011	0.304568
H	-3.016225	-2.407839	0.757430
C	-2.596918	1.741162	-0.189502
C	-2.883617	2.216376	1.113509
C	-3.382837	3.522305	1.253140
C	-3.603120	4.348912	0.151905
C	-3.323455	3.876434	-1.131727
C	-2.826070	2.583773	-1.295239
H	-2.620661	2.237392	-2.309064
H	-3.494149	4.508356	-2.006350
H	-3.994954	5.358707	0.295756
H	-3.606351	3.894084	2.256926
C	-2.629753	1.411056	2.370918
C	-1.187869	1.553832	2.871290
H	-0.462849	1.167948	2.126306
H	-0.920768	2.610606	3.026014
H	-1.026621	1.012472	3.815220
H	-2.868034	0.347920	2.214097
H	-3.312576	1.760136	3.160887
C	-1.039811	0.142261	-2.079939
C	0.203741	1.030376	-1.933427
P	1.361951	0.491981	-0.566100
C	2.268512	2.041652	-0.193435
C	2.178450	2.624828	1.078851
C	2.865413	3.809438	1.362059
C	3.644733	4.418531	0.374763
C	3.739693	3.841009	-0.897006
C	3.058595	2.655795	-1.180727
H	3.157313	2.197763	-2.168274
H	4.354152	4.311816	-1.668266
H	4.184455	5.342410	0.596777
H	2.794153	4.253971	2.357652
H	1.580462	2.150871	1.860101
C	2.606153	-0.614932	-1.352333
C	2.414954	-1.089248	-2.662932
C	3.306792	-1.995457	-3.238117
C	4.406199	-2.442394	-2.502055
C	4.596404	-1.984385	-1.198270
C	3.709948	-1.078152	-0.594653
C	3.989580	-0.643694	0.830594
C	5.144033	0.360033	0.951290
H	4.931961	1.282703	0.391765
H	6.078717	-0.066965	0.554780
H	5.316842	0.631344	2.004894
H	4.227608	-1.541241	1.426480
H	3.085355	-0.212107	1.288017
H	5.451247	-2.346323	-0.619979
H	5.111123	-3.153294	-2.939857
H	3.139816	-2.350793	-4.257638
H	1.559171	-0.759637	-3.254056
H	0.746836	1.114927	-2.887002
H	-0.092518	2.053618	-1.655339
H	-0.781790	-0.892056	-2.352755
H	-1.695141	0.517833	-2.879534
C	-0.903653	-1.866601	2.665501
C	0.564811	-1.959529	2.987885
C	1.215154	-3.349461	2.979449
C	0.904307	-4.215688	1.751081
H	-0.143206	-4.561971	1.786926
H	1.519660	-5.127238	1.825717
C	1.159878	-3.542820	0.394018
C	0.071297	-2.579088	-0.083174
H	-0.912802	-3.077973	-0.095543
H	0.291790	-2.252265	-1.112247
H	1.260188	-4.339895	-0.367197
H	2.143158	-3.039038	0.402316
H	0.888244	-3.877653	3.890982
H	2.308511	-3.224772	3.068927
H	0.837627	-1.409541	3.903658
H	1.192555	-1.355888	2.212397
H	-1.404813	-2.824594	2.484072
H	-1.486629	-1.243086	3.356086

^{4}5C-09
Geometry with 83 atoms:
Total energy: -3124.210726580

Cr	0.044026	-1.032149	0.835402
P	-1.744961	0.186892	-0.609698
C	-3.054256	-0.863565	-1.344073
C	-2.738151	-1.724705	-2.410953
C	-3.699754	-2.602746	-2.917358
C	-4.983493	-2.635596	-2.363278
C	-5.304539	-1.780831	-1.304343
C	-4.347645	-0.898633	-0.794743
H	-4.615782	-0.226792	0.023485
H	-6.309163	-1.793993	-0.874608
H	-5.734138	-3.322918	-2.760641
H	-3.444339	-3.262256	-3.750372
H	-1.741482	-1.713344	-2.859177
C	-2.615221	1.643555	0.094925
C	-2.632899	1.897458	1.487744
C	-3.285213	3.057677	1.939912
C	-3.904239	3.942399	1.056279
C	-3.889774	3.681320	-0.316751
C	-3.248490	2.537230	-0.788926
H	-3.243765	2.335137	-1.863112
H	-4.374815	4.365226	-1.017043
H	-4.400723	4.836635	1.440937
H	-3.306184	3.267546	3.012819
C	-2.047818	0.953518	2.520394

C -2.951883 -0.245260 2.833574
H -3.163622 -0.840257 1.931527
H -2.487968 -0.906930 3.582056
H -3.918805 0.095128 3.235410
H -1.847970 1.512113 3.447715
H -1.050260 0.596195 2.192703
C -0.788659 0.865723 -2.074088
C 0.578865 0.189601 -2.257771
P 1.539367 0.222871 -0.661120
C 1.752002 2.028650 -0.416577
C 1.037374 2.688311 0.594577
C 1.131967 4.076014 0.735003
C 1.944938 4.811174 -0.132006
C 2.663198 4.158336 -1.141019
C 2.568063 2.772688 -1.285560
H 3.140431 2.267524 -2.068330
H 3.303703 4.731396 -1.815831
H 2.022680 5.895411 -0.020829
H 0.568353 4.580411 1.523350
H 0.400166 2.125561 1.280202
C 3.190388 -0.488499 -1.009919
C 3.409432 -1.194929 -2.208513
C 4.628283 -1.827709 -2.453460
C 5.642603 -1.765542 -1.495190
C 5.430570 -1.066784 -0.306732
C 4.215863 -0.417108 -0.034464
C 4.087728 0.348041 1.267914
C 4.902117 1.648149 1.290336
H 4.789721 2.158959 2.259893
H 4.571510 2.340274 0.501779
H 5.974540 1.449867 1.135646
H 4.422035 -0.305166 2.090623
H 3.034571 0.576925 1.482647
H 6.226907 -1.023359 0.441562
H 6.598964 -2.263740 -1.672278
H 4.781815 -2.368841 -3.390010
H 2.629671 -1.261491 -2.968198
H 0.464541 -0.863201 -2.557443
H 1.156204 0.704172 -3.042160
H -1.392110 0.765427 -2.988535
H -0.657489 1.941738 -1.885624
C 0.034359 -2.741384 -0.217207
C -0.959669 -3.184934 0.829932
C -0.540425 -4.310255 1.783968
C 0.797073 -4.106388 2.510881
H 1.636293 -4.227787 1.803582
H 0.903240 -4.924678 3.241942
C 0.946356 -2.752756 3.225556
C 1.357029 -1.598046 2.303365
H 2.333627 -1.818229 1.839062
H 1.484499 -0.660259 2.886192
H 1.705664 -2.866718 4.022485
H 0.005968 -2.515631 3.761094
H -0.502533 -5.247204 1.202613
H -1.341135 -4.442987 2.532508
H -1.947948 -3.393891 0.388765
H -1.234028 -2.300934 1.517034
H 1.003371 -3.256457 -0.205331
H -0.373395 -2.678513 -1.234071

^{45}C-10
Geometry with 83 atoms:
Total energy: -3124.210541600
Cr -0.103001 -1.043907 0.870113
P -1.932104 -0.133646 -0.517615
C -3.457921 -1.099102 -0.810323
C -4.493024 -0.590584 -1.614701
C -5.638617 -1.354494 -1.843040
C -5.762450 -2.625080 -1.268009
C -4.740110 -3.130517 -0.460456
C -3.589573 -2.370524 -0.229086
H -2.795705 -2.762477 0.409233
H -4.837831 -4.118788 -0.004715
H -6.662323 -3.218797 -1.446691
H -6.441252 -0.955295 -2.467890
H -4.413157 0.407284 -2.053207
C -2.480218 1.586611 -0.128453
C -2.751079 1.971329 1.207237
C -3.141414 3.298192 1.454037
C -3.272549 4.229989 0.424615
C -3.022661 3.842474 -0.893478
C -2.634177 2.530237 -1.162953
H -2.449750 2.252712 -2.201526
H -3.131058 4.556923 -1.712692
H -3.576953 5.254854 0.650329
H -3.351038 3.601104 2.483751
C -2.585463 1.042148 2.392101
C -1.196081 1.148907 3.031019
H -0.385203 0.872605 2.329106
H -0.979841 2.183587 3.339406
H -1.106462 0.502203 3.916156
H -2.791792 -0.000603 2.106531
H -3.339775 1.300704 3.151747
C -1.103978 -0.008869 -2.180723
C 0.165669 0.854396 -2.133022
P 1.294950 0.522031 -0.668582
C 1.861619 2.224175 -0.274092
C 0.998938 3.046502 0.472470
C 1.351063 4.368617 0.751166
C 2.569815 4.880018 0.292318
C 3.428551 4.068449 -0.455413
C 3.077375 2.745586 -0.743053
H 3.751680 2.122663 -1.334421
H 4.377876 4.466699 -0.822108
H 2.848520 5.913113 0.514034
H 0.670320 4.999416 1.328046
H 0.038387 2.662513 0.823054
C 2.769954 -0.404071 -1.260060
C 2.821002 -0.908317 -2.572172
C 3.880437 -1.710084 -2.997495
C 4.909398 -2.021436 -2.106428
C 4.863106 -1.532091 -0.801296
C 3.805922 -0.727062 -0.346684
C 3.826885 -0.276734 1.103545
C 5.010064 0.630099 1.465422
H 5.974190 0.135758 1.269423
H 4.981502 0.894457 2.534416
H 4.986478 1.564677 0.885574
H 3.856117 -1.178960 1.740183
H 2.894368 0.243966 1.365503
H 5.663444 -1.791802 -0.103378
H 5.743480 -2.651576 -2.424520
H 3.897429 -2.090761 -4.021270
H 2.023465 -0.686337 -3.282141
H 0.719605 0.795124 -3.081236
H -0.107341 1.911781 -2.010807
H -0.888040 -1.048896 -2.467272
H -1.810135 0.376094 -2.932694
C -0.744687 -2.195057 2.418660
C 0.729026 -2.215595 2.733320
C 1.460968 -3.561140 2.645688
C 1.215607 -4.353884 1.354885
H 0.191670 -4.766127 1.350167
H 1.885847 -5.228993 1.371043
C 1.444909 -3.565638 0.056763
C 0.302757 -2.640531 -0.371746
H -0.645899 -3.200993 -0.445907
H 0.522204 -2.227342 -1.369977
H 1.610830 -4.293996 -0.759592
H 2.390915 -2.999373 0.125423
H 1.156698 -4.168262 3.514845
H 2.544330 -3.378584 2.758332
H 0.970794 -1.701624 3.678171
H 1.316311 -1.540022 1.989611
H -1.179340 -3.167847 2.158059
H -1.368602 -1.674294 3.156746

^{45}C-11
Geometry with 83 atoms:
Total energy: -3124.208443480
Cr 0.235885 -0.804485 1.068331
P -1.667968 0.067109 -0.280726
C -2.627249 -1.325896 -0.974212
C -2.539558 -1.724609 -2.315676
C -3.240040 -2.851566 -2.758294
C -4.025110 -3.587577 -1.867071
C -4.108281 -3.197574 -0.525239
C -3.408972 -2.076172 -0.077575
H -3.474719 -1.779795 0.972917
H -4.720168 -3.770262 0.175868
H -4.571279 -4.467162 -2.216119
H -3.169890 -3.154225 -3.805874
H -1.928830 -1.166146 -3.028310
C -2.846919 1.215532 0.535448
C -3.970071 1.797221 -0.103704
C -4.732828 2.722336 0.630115
C -4.418912 3.067507 1.944840
C -3.319384 2.479469 2.574370
C -2.544746 1.560344 1.867967
H -1.695836 1.088579 2.366924
H -3.067379 2.730496 3.607228
H -5.035961 3.794569 2.478597
H -5.598772 3.184493 0.147746
C -4.432348 1.455562 -1.505996
C -5.661325 0.535087 -1.518790
H -5.976116 0.323729 -2.552967
H -5.442884 -0.424623 -1.027331
H -6.511366 0.998359 -0.993287
H -3.629747 0.982589 -2.084769
H -4.677077 2.393989 -2.031341
C -0.927133 1.032767 -1.698099
C 0.493578 0.589666 -2.074689
P 1.624662 0.597936 -0.588858
C 1.792678 2.392680 -0.228094
C 2.795396 3.180828 -0.817077
C 2.862477 4.549643 -0.543916
C 1.930556 5.145097 0.313060
C 0.930219 4.367248 0.903851
C 0.865169 2.996458 0.640382
H 0.076331 2.404539 1.113152
H 0.199272 4.824863 1.574905
H 1.986378 6.216096 0.522619
H 3.647265 5.154673 -1.004645
H 3.528313 2.725390 -1.487323
C 3.261541 0.038868 -1.197564
C 3.443383 -0.321219 -2.546638
C 4.680851 -0.771633 -3.007469
C 5.758046 -0.855838 -2.122414
C 5.585104 -0.499200 -0.784857
C 4.347064 -0.057203 -0.291926
C 4.232334 0.272834 1.184174
C 4.422949 -0.950802 2.089326
H 4.273575 -0.685450 3.148097
H 5.435394 -1.371163 1.990422
H 3.713028 -1.751211 1.830583
H 3.261427 0.741469 1.404562
H 4.985854 1.037737 1.437790
H 6.433805 -0.563775 -0.098385
H 6.734619 -1.197427 -2.474141
H 4.802443 -1.048030 -4.057408
H 2.619980 -0.250413 -3.258312
H 0.493419 -0.432997 -2.483709
H 0.899120 1.259524 -2.848849
H -1.583514 0.997256 -2.579546
H -0.922197 2.079277 -1.356246
C -0.600207 -1.649364 2.713961
C 0.844486 -1.896910 3.063864
C 1.348162 -3.345167 3.097583
C 1.026431 -4.188683 1.855893
H -0.051403 -4.425890 1.826582
H 1.540304 -5.156785 1.973276
C 1.429361 -3.558507 0.512274
C 0.446301 -2.525073 -0.035654
H -0.572224 -2.944892 -0.089793
H 0.734613 -2.210668 -1.053892
H 1.513272 -4.372147 -0.233463
H 2.448520 -3.134052 0.584793
H 0.917444 -3.829136 3.990207
H 2.440989 -3.329183 3.251329
H 1.158869 -1.359662 3.974028
H 1.542658 -1.377149 2.289157
H -1.204587 -2.545801 2.527410
H -1.122607 -0.954560 3.388397

^{45}C-12
Geometry with 83 atoms:
Total energy: -3124.210505470
Cr -0.152827 -0.577820 1.163809
P -1.961666 0.081724 -0.428713
C -3.251855 -1.184125 -0.715126
C -3.694901 -1.542493 -1.998901
C -4.697054 -2.505275 -2.149801
C -5.265780 -3.111812 -1.025945

C	-4.827731	-2.758586	0.254713
C	-3.821393	-1.803325	0.410859
H	-3.468018	-1.544699	1.412399
H	-5.265821	-3.234555	1.135257
H	-6.049326	-3.863628	-1.148325
H	-5.034512	-2.781465	-3.151823
H	-3.266016	-1.080762	-2.890447
C	-2.883137	1.686433	-0.335370
C	-3.020945	2.429802	0.860953
C	-3.747381	3.632720	0.814176
C	-4.339243	4.091737	-0.361685
C	-4.225484	3.338919	-1.533097
C	-3.506294	2.145491	-1.511873
H	-3.447480	1.557464	-2.429806
H	-4.700692	3.673539	-2.458132
H	-4.899860	5.029700	-0.360524
H	-3.856652	4.215205	1.733128
C	-2.410757	2.008189	2.180523
C	-0.932582	2.389580	2.308109
H	-0.325073	1.932603	1.505153
H	-0.785416	3.476383	2.209259
H	-0.516907	2.076095	3.279123
H	-2.527934	0.923889	2.323168
H	-2.972984	2.483212	2.999164
C	-1.018448	0.206856	-2.029752
C	0.217407	1.103665	-1.876160
P	1.411982	0.486269	-0.584222
C	2.451994	1.959789	-0.252160
C	2.540176	2.480949	1.047933
C	3.341067	3.596882	1.308238
C	4.057034	4.200173	0.270515
C	3.974433	3.685188	-1.028630
C	3.179016	2.567817	-1.289923
H	3.138353	2.157154	-2.302104
H	4.539109	4.151535	-1.839562
H	4.685289	5.070695	0.474282
H	3.408964	3.991997	2.324708
H	1.995496	2.009138	1.868965
C	2.519468	-0.717022	-1.429700
C	2.240327	-1.148472	-2.739522
C	3.024405	-2.122046	-3.360119
C	4.102589	-2.681964	-2.671807
C	4.385221	-2.260135	-1.372706
C	3.611330	-1.283652	-0.725730
C	4.011014	-0.868934	0.675912
C	5.229237	0.064261	0.710910
H	6.107835	-0.421345	0.257696
H	5.486773	0.330142	1.748510
H	5.037283	0.995492	0.158458
H	4.236184	-1.777555	1.259196
H	3.167867	-0.383184	1.190351
H	5.228356	-2.701897	-0.834064
H	4.721207	-3.448552	-3.144670
H	2.790128	-2.440624	-4.378565
H	1.404146	-0.728017	-3.299113
H	0.727317	1.247108	-2.841153
H	-0.080316	2.108011	-1.532352
H	-0.743458	-0.822401	-2.306510
H	-1.662408	0.593482	-2.832473
C	-0.845229	-1.248315	2.950638
C	0.627116	-1.419742	3.216054
C	1.164055	-2.846291	3.395022
C	0.731926	-3.853843	2.320794
H	-0.338191	-4.098303	2.436595
H	1.272636	-4.794808	2.514651
C	0.988568	-3.410027	0.873066
C	-0.040298	-2.439149	0.290976
H	-1.059589	-2.852498	0.381643
H	0.165525	-2.270202	-0.779821
H	0.995652	-4.313651	0.234137
H	2.009211	-2.995939	0.785282
H	0.837439	-3.204539	4.385825
H	2.266782	-2.803296	3.429107
H	0.992722	-0.765072	4.024439
H	1.257579	-0.995603	2.329742
H	-1.434788	-2.172690	2.935022
H	-1.330525	-0.479254	3.568486

^{4}5C-13
Geometry with 83 atoms:
Total energy: -3124.207988990

Cr	0.003947	-0.633935	1.059725
P	-1.883554	0.091820	-0.536507
C	-3.233996	-1.096611	-0.869966
C	-4.368781	-1.073819	-0.037522
C	-5.372475	-2.031863	-0.186740
C	-5.256397	-3.026025	-1.165082
C	-4.133147	-3.054520	-1.995011
C	-3.123581	-2.097144	-1.849895
H	-2.254820	-2.142538	-2.508688
H	-4.038182	-3.825386	-2.763758
H	-6.042655	-3.775982	-1.280389
H	-6.250823	-2.001370	0.462653
H	-4.475879	-0.296348	0.723964
C	-2.718310	1.729968	-0.399468
C	-2.400471	2.669872	0.608473
C	-3.069978	3.907270	0.593505
C	-4.021992	4.215479	-0.377294
C	-4.332889	3.281000	-1.369850
C	-3.682597	2.049159	-1.376144
H	-3.934609	1.317419	-2.148009
H	-5.078386	3.510110	-2.134836
H	-4.522746	5.186568	-0.359494
H	-2.834863	4.643522	1.366987
C	-1.433606	2.398551	1.743902
C	-2.093385	1.688626	2.933428
H	-1.370188	1.515346	3.746352
H	-2.916428	2.297516	3.337954
H	-2.523755	0.717347	2.638492
H	-1.010046	3.355974	2.085853
H	-0.558774	1.830137	1.381874
C	-0.921910	0.253396	-2.124216
C	0.282088	1.181540	-1.911548
P	1.463353	0.548435	-0.611892
C	2.421914	2.041981	-0.159833
C	3.219053	2.684826	-1.122427
C	3.921992	3.843852	-0.787135
C	3.838675	4.365882	0.508952
C	3.055607	3.723719	1.472518
C	2.350631	2.562987	1.140909
H	1.757260	2.055643	1.904412
H	2.998045	4.122550	2.488185
H	4.391913	5.271667	0.769077
H	4.541266	4.339020	-1.539039
H	3.300684	2.273830	-2.132207
C	2.632177	-0.572254	-1.483722
C	2.391426	-0.958506	-2.813817
C	3.223480	-1.877610	-3.455879
C	4.307129	-2.420586	-2.765594
C	4.552667	-2.041320	-1.443949
C	3.733679	-1.119678	-0.774653
C	4.038261	-0.701508	0.650458
C	4.734609	-1.740811	1.528809
H	4.177846	-2.691986	1.543678
H	4.805513	-1.372658	2.564108
H	5.761007	-1.957055	1.194521
H	3.098478	-0.410406	1.141344
H	4.642421	0.223038	0.619522
H	5.406633	-2.476202	-0.922404
H	4.965672	-3.142816	-3.254301
H	3.021118	-2.165488	-4.490134
H	1.547939	-0.550530	-3.371568
H	0.819097	1.368629	-2.853595
H	-0.049941	2.166714	-1.545869
H	-0.594884	-0.756622	-2.415722
H	-1.578285	0.637860	-2.920847
C	1.062384	-0.881691	2.758014
C	-0.197428	-1.563350	3.248571
C	-0.119921	-3.081334	3.495927
C	-0.273793	-3.973419	2.255746
H	-1.326906	-3.944417	1.918558
H	-0.089863	-5.013578	2.571512
C	0.626800	-3.643453	1.054000
C	0.140152	-2.485792	0.182541
H	-0.881083	-2.697496	-0.185954
H	0.799724	-2.354192	-0.690879
H	0.675807	-4.545341	0.413926
H	1.664131	-3.470804	1.390652
H	-0.900797	-3.363590	4.220926
H	0.845947	-3.287988	3.987057
H	-1.064153	-1.420079	2.492868
H	-0.627005	-1.041705	4.119041
H	1.293896	0.065004	3.272107
H	1.950541	-1.523580	2.718582

^{4}5C-14
Geometry with 83 atoms:
Total energy: -3124.208436480

Cr	0.201732	-0.890121	1.017910
P	1.676319	0.491463	-0.435540
C	1.351293	2.264569	-0.084496
C	1.073102	2.657154	1.236417
C	0.780226	3.990768	1.534853
C	0.762474	4.947101	0.516701
C	1.056075	4.570345	-0.798447
C	1.353556	3.239585	-1.098741
H	1.591829	2.970215	-2.129970
H	1.055559	5.317822	-1.595483
H	0.526350	5.988776	0.747087
H	0.564183	4.279934	2.566042
H	1.094423	1.924594	2.046054
C	3.504497	0.325663	-0.558874
C	4.114581	-0.910913	-0.882369
C	5.517579	-0.971456	-0.902202
C	6.306906	0.139936	-0.608522
C	5.698260	1.354030	-0.281771
C	4.307068	1.443012	-0.254438
H	3.844409	2.394696	0.009759
H	6.302656	2.232435	-0.043791
H	7.396254	0.056502	-0.628734
H	5.997392	-1.922567	-1.149785
C	3.337036	-2.159429	-1.238112
C	3.371039	-2.489461	-2.736664
H	2.975768	-1.658809	-3.342831
H	4.400430	-2.680089	-3.078580
H	2.772918	-3.389134	-2.954073
H	2.296057	-2.068833	-0.899156
H	3.755549	-3.009279	-0.673570
C	0.954923	0.227528	-2.137118
C	-0.528475	0.622514	-2.198632
P	-1.527181	-0.006152	-0.736732
C	-2.659958	-1.266661	-1.434261
C	-2.177395	-2.207656	-2.362086
C	-3.005782	-3.235398	-2.820327
C	-4.319910	-3.340848	-2.353436
C	-4.805311	-2.409727	-1.430194
C	-3.982551	-1.377453	-0.970663
H	-4.379013	-0.648425	-0.260368
H	-5.833846	-2.481217	-1.068035
H	-4.965950	-4.145510	-2.712432
H	-2.621603	-3.956746	-3.545678
H	-1.153291	-2.145065	-2.739297
C	-2.603442	1.417642	-0.290342
C	-3.267833	2.094453	-1.331385
C	-4.059398	3.211717	-1.073517
C	-4.194903	3.666814	0.241400
C	-3.551125	2.994527	1.279631
C	-2.751336	1.861922	1.044389
C	-2.172922	1.136921	2.242458
C	-3.041777	-0.043294	2.695546
H	-2.593400	-0.562058	3.557533
H	-3.180905	-0.775578	1.884976
H	-4.041968	0.307395	2.993857
H	-2.056985	1.848852	3.074142
H	-1.141290	0.792736	2.030905
H	-3.669527	3.352391	2.306139
H	-4.806530	4.545723	0.459632
H	-4.566481	3.724917	-1.893865
H	-3.167581	1.738914	-2.360184
H	-0.634840	1.715649	-2.191903
H	-0.983671	0.259060	-3.132140
H	1.540637	0.780128	-2.888241
H	1.083949	-0.841875	-2.357134
C	0.178252	-2.804438	0.392725
C	-0.867475	-2.960465	1.469964
C	-0.508092	-3.824656	2.685252
C	0.823750	-3.492576	3.374955
H	1.669673	-3.804793	2.737638
H	0.888695	-4.119255	4.279598
C	1.015959	-2.015761	3.760121
C	1.476679	-1.107241	2.611354
H	2.456673	-1.443052	2.225495
H	1.631912	-0.072582	2.982466

H	1.761801	-1.970926	4.576231
H	0.079103	-1.630714	4.209483
H	-0.494351	-4.877517	2.355915
H	-1.326889	-3.742119	3.421474
H	-1.843856	-3.256425	1.052894
H	-1.147780	-1.934712	1.905133
H	1.117543	-3.341100	0.572747
H	-0.186070	-2.961715	-0.630744

^{4}5C-15
Geometry with 83 atoms:
Total energy: -3124.205982690

Cr	0.075569	-0.811099	0.978340
P	1.622622	0.336724	-0.609242
C	2.189256	2.044422	-0.249903
C	1.781354	2.712208	0.913531
C	2.206337	4.022725	1.155660
C	3.039463	4.669938	0.239528
C	3.450192	4.006496	-0.923033
C	3.029201	2.698597	-1.168612
H	3.372095	2.180541	-2.068233
H	4.107740	4.507676	-1.637463
H	3.374554	5.692078	0.431866
H	1.888300	4.535740	2.066465
H	1.142532	2.208352	1.639105
C	3.108830	-0.586664	-1.149733
C	4.164965	-0.807840	-0.231230
C	5.262212	-1.570638	-0.661080
C	5.327331	-2.106714	-1.947561
C	4.279896	-1.887334	-2.845323
C	3.176434	-1.132741	-2.445529
H	2.368021	-0.973854	-3.160854
H	4.318717	-2.301155	-3.855652
H	6.194980	-2.699128	-2.248204
H	6.082532	-1.750503	0.039528
C	4.183873	-0.242439	1.175826
C	5.139459	0.946480	1.343969
H	6.174434	0.659734	1.098889
H	4.858545	1.783244	0.688125
H	5.126496	1.309878	2.383773
H	4.484676	-1.046787	1.867830
H	3.171374	0.054816	1.489351
C	0.571083	0.600140	-2.126085
C	-0.704765	1.372696	-1.760847
P	-1.727878	0.402663	-0.539075
C	-2.432052	-0.918619	-1.604526
C	-1.988770	-2.238288	-1.422807
C	-2.474540	-3.269713	-2.232121
C	-3.413600	-2.985352	-3.227578
C	-3.863049	-1.672079	-3.413856
C	-3.375527	-0.641450	-2.607610
H	-3.742854	0.378630	-2.748492
H	-4.601246	-1.451857	-4.188844
H	-3.800463	-3.789298	-3.858419
H	-2.123815	-4.293370	-2.081228
H	-1.261206	-2.473771	-0.634998
C	-3.130669	1.488265	-0.067950
C	-3.189834	2.821365	-0.518033
C	-4.219944	3.670549	-0.112051
C	-5.206476	3.195053	0.754773
C	-5.155345	1.874840	1.202638
C	-4.131469	0.999011	0.808767
C	-4.176118	-0.431646	1.306010
C	-5.233926	-1.289962	0.599006
H	-5.044819	-1.346184	-0.483104
H	-6.242413	-0.871196	0.742998
H	-5.233852	-2.316420	0.999256
H	-4.382673	-0.422820	2.389498
H	-3.191164	-0.908129	1.190156
H	-5.929561	1.505733	1.881316
H	-6.015397	3.852240	1.083119
H	-4.248978	4.700921	-0.474047
H	-2.432284	3.214522	-1.196816
H	-0.445399	2.338746	-1.299738
H	-1.300345	1.580670	-2.663364
H	1.152764	1.150586	-2.882014
H	0.321383	-0.385697	-2.549881
C	1.238579	-2.469536	1.249657
C	0.788533	-3.500331	2.288191
C	0.759319	-2.960108	3.728241
C	-0.511309	-2.178282	4.091278
H	-0.397458	-1.738108	5.096459
H	-1.358979	-2.882624	4.155588
C	-0.900899	-1.048549	3.130100
C	0.140265	-0.003452	2.812637
H	1.090871	-0.087359	3.354889
H	-0.243522	1.027181	2.815429
H	-1.860081	-0.597530	3.430908
H	-1.232754	-1.574415	2.159261
H	1.653514	-2.333099	3.890997
H	0.847501	-3.796175	4.441167
H	1.474035	-4.368175	2.254625
H	-0.206734	-3.912948	2.031081
H	2.286596	-2.180882	1.428213
H	1.199768	-2.890528	0.220007

^{4}5C-16
Geometry with 83 atoms:
Total energy: -3124.210026070

Cr	-0.042492	-1.019759	0.854472
P	-1.921001	-0.193811	-0.526961
C	-3.401304	-1.227405	-0.819141
C	-4.486336	-0.745279	-1.572438
C	-5.596332	-1.561004	-1.797835
C	-5.635044	-2.857350	-1.270381
C	-4.563168	-3.336948	-0.512812
C	-3.448134	-2.525106	-0.284415
H	-2.616094	-2.896232	0.316318
H	-4.594349	-4.345478	-0.093539
H	-6.507366	-3.491596	-1.446409
H	-6.438050	-1.182161	-2.382659
H	-4.474278	0.271902	-1.971494
C	-2.542661	1.486109	-0.077546
C	-2.773800	1.828495	1.277590
C	-3.212961	3.129952	1.571822
C	-3.429236	4.077314	0.570844
C	-3.217355	3.731142	-0.765132
C	-2.781150	2.444404	-1.081654
H	-2.627006	2.198949	-2.133246
H	-3.391663	4.457663	-1.561986
H	-3.770024	5.081752	0.833383
H	-3.393231	3.400591	2.616006
C	-2.519697	0.879328	2.431768
C	-1.091325	0.980512	2.980255
H	-0.328630	0.735746	2.209665
H	-0.855594	2.008453	3.295571
H	-0.934231	0.311518	3.838206
H	-2.738834	-0.159369	2.142145
H	-3.221039	1.119343	3.246070
C	-1.115584	0.019397	-2.191174
C	0.097109	0.960105	-2.126671
P	1.258005	0.660138	-0.680069
C	1.733240	2.381590	-0.249548
C	2.925057	2.970893	-0.700103
C	3.211040	4.302933	-0.385783
C	2.309224	5.058650	0.369981
C	1.115462	4.479414	0.812858
C	0.829802	3.146348	0.509528
H	-0.111465	2.711529	0.852681
H	0.401396	5.065305	1.396806
H	2.535475	6.100261	0.610820
H	4.141858	4.753394	-0.739304
H	3.631909	2.391827	-1.298902
C	2.772782	-0.162215	-1.318154
C	2.810516	-0.668177	-2.628188
C	3.904828	-1.402883	-3.087877
C	4.979501	-1.639702	-2.231366
C	4.948697	-1.148517	-0.924251
C	3.859146	-0.411893	-0.435271
C	3.857948	0.100020	0.993673
C	4.716182	-0.675692	1.992641
H	5.791906	-0.573742	1.783267
H	4.474641	-1.750887	1.988028
H	4.550126	-0.293695	3.011913
H	2.818061	0.120301	1.362138
H	4.168474	1.159396	0.991183
H	5.794636	-1.354255	-0.267070
H	5.843436	-2.213494	-2.575499
H	3.911034	-1.788814	-4.109778
H	1.975154	-0.504339	-3.309959
H	0.648759	0.959522	-3.078228
H	-0.240425	1.994821	-1.976556
H	-0.833894	-0.998311	-2.500562
H	-1.846741	0.375009	-2.933439
C	-0.637992	-2.288604	2.323614
C	0.828107	-2.250003	2.669676
C	1.636580	-3.545571	2.518821
C	1.455084	-4.282820	1.185546
H	0.459405	-4.757999	1.146695
H	2.179196	-5.113851	1.166179
C	1.645451	-3.416981	-0.068729
C	0.451385	-2.542104	-0.458979
H	-0.461626	-3.154946	-0.560255
H	0.645629	-2.080395	-1.440357
H	1.859182	-4.092187	-0.918933
H	2.556810	-2.800832	0.035388
H	1.355369	-4.214536	3.349480
H	2.705285	-3.307657	2.660379
H	1.020693	-1.786580	3.651329
H	1.387224	-1.489967	1.989129
H	-1.012378	-3.266331	1.997906
H	-1.304358	-1.850429	3.078605

^{4}5C-17
Geometry with 83 atoms:
Total energy: -3124.208142490

Cr	-0.051066	-0.270899	1.208436
P	-1.822052	0.049747	-0.641030
C	-3.111783	-1.235160	-0.822164
C	-2.823915	-2.469655	-1.431176
C	-3.775995	-3.492858	-1.434048
C	-5.019080	-3.301189	-0.823949
C	-5.310600	-2.077208	-0.212963
C	-4.364799	-1.049585	-0.209551
H	-4.610278	-0.095909	0.264218
H	-6.282031	-1.918454	0.261755
H	-5.760838	-4.103475	-0.826615
H	-3.542116	-4.445215	-1.916064
H	-1.856551	-2.649568	-1.904758
C	-2.704144	1.663760	-0.775105
C	-2.477695	2.733107	0.122138
C	-3.158857	3.943542	-0.102860
C	-4.040670	4.100688	-1.170746
C	-4.265655	3.037507	-2.051389
C	-3.597516	1.831863	-1.851955
H	-3.777410	1.001601	-2.539876
H	-4.956482	3.148193	-2.890402
H	-4.553201	5.054592	-1.317506
H	-2.989363	4.778605	0.582489
C	-1.602933	2.633688	1.356097
C	-2.377465	2.165346	2.593324
H	-1.717346	2.072692	3.470066
H	-3.171839	2.885675	2.842027
H	-2.865664	1.192338	2.422221
H	-1.153618	3.618391	1.560474
H	-0.732397	1.977201	1.160257
C	-0.809184	0.019857	-2.201387
C	0.442015	0.888986	-2.019687
P	1.528714	0.307883	-0.620196
C	2.722936	1.679199	-0.420219
C	3.698107	1.918509	-1.403949
C	4.586737	2.985625	-1.261530
C	4.512617	3.816100	-0.136994
C	3.546352	3.580020	0.844903
C	2.652173	2.513996	0.705908
H	1.910953	2.327114	1.485958
H	3.491642	4.222463	1.727023
H	5.214216	4.646358	-0.024993
H	5.344976	3.165862	-2.027386
H	3.773771	1.261482	-2.274212
C	2.480134	-1.118517	-1.300175
C	2.247934	-1.566942	-2.615191
C	2.922527	-2.674912	-3.129305
C	3.844825	-3.353683	-2.330242
C	4.088292	-2.909608	-1.031107
C	3.423856	-1.797108	-0.490078
C	3.785684	-1.354352	0.909565
C	5.134820	-0.626837	0.985624
H	5.956017	-1.273405	0.637378
H	5.355702	-0.328775	2.022945
H	5.135125	0.280733	0.363548
H	3.814009	-2.240972	1.564936
H	2.999878	-0.706871	1.316558

H	4.815608	-3.437247	-0.407679
H	4.375452	-4.226296	-2.718879
H	2.726256	-3.002834	-4.152797
H	1.540770	-1.054083	-3.266464
H	1.028017	0.959481	-2.948973
H	0.162612	1.922343	-1.755483
H	-0.539198	-1.025798	-2.407091
H	-1.417169	0.377692	-3.046615
C	1.065835	0.012793	2.910227
C	0.970769	-1.191765	3.853681
C	-0.480781	-1.575413	4.178030
C	-1.409497	-1.689509	2.961533
H	-1.572848	-0.662530	2.525021
H	-2.431854	-1.913385	3.306784
C	-1.025458	-2.724454	1.870034
C	0.108498	-2.269549	0.946643
H	-0.014397	-2.610090	-0.092863
H	1.114063	-2.549028	1.292867
H	-1.923911	-2.922497	1.265272
H	-0.778728	-3.671519	2.383261
H	-0.907657	-0.819094	4.860540
H	-0.506489	-2.533113	4.725770
H	1.499037	-0.993541	4.805445
H	1.493831	-2.054158	3.405058
H	0.553492	0.892252	3.361952
H	2.113111	0.312242	2.749140

[4]5C-18

Geometry with 83 atoms:

Total energy: -3124.207071100

Cr	-0.002189	-0.697004	0.955382
P	1.696205	0.224281	-0.625849
C	2.268873	1.963831	-0.524619
C	3.360794	2.388052	-1.302670
C	3.762819	3.724664	-1.274736
C	3.080829	4.647391	-0.472883
C	1.993555	4.230910	0.299651
C	1.586323	2.893019	0.275772
H	0.741527	2.578999	0.889034
H	1.460314	4.947328	0.929193
H	3.401012	5.691851	-0.449371
H	4.615509	4.046408	-1.877635
H	3.906951	1.671792	-1.921766
C	3.197440	-0.796750	-0.875467
C	4.109437	-0.954419	0.197863
C	5.221441	-1.788243	0.002289
C	5.439656	-2.451402	-1.205855
C	4.537209	-2.289509	-2.259659
C	3.422242	-1.466793	-2.092966
H	2.731795	-1.353619	-2.929855
H	4.698186	-2.800984	-3.211583
H	6.313663	-3.096529	-1.324029
H	5.929911	-1.919339	0.824862
C	3.961193	-0.243645	1.528406
C	4.947085	0.918096	1.710965
H	4.809275	1.392671	2.695546
H	5.989605	0.567843	1.647776
H	4.804983	1.689232	0.939448
H	4.115682	-0.979893	2.334958
H	2.932090	0.124549	1.657048
C	0.770811	0.217267	-2.248773
C	-0.549490	0.992145	-2.124753
P	-1.640970	0.215095	-0.828289
C	-2.277880	-1.285067	-1.679997
C	-3.335186	-1.235071	-2.602995
C	-3.756626	-2.400222	-3.248810
C	-3.125811	-3.621559	-2.984751
C	-2.074432	-3.681569	-2.065019
C	-1.657199	-2.518403	-1.412365
H	-0.846705	-2.584866	-0.675649
H	-1.584304	-4.634053	-1.849248
H	-3.459554	-4.529760	-3.492492
H	-4.583795	-2.355781	-3.961598
H	-3.837794	-0.286443	-2.809316
C	-3.067751	1.334330	-0.591246
C	-3.193038	2.513806	-1.346323
C	-4.253800	3.394607	-1.125821
C	-5.198241	3.099410	-0.142680
C	-5.083056	1.927372	0.609886
C	-4.031464	1.022498	0.406708
C	-3.935143	-0.264627	1.202742
C	-4.755835	-0.341945	2.487545
H	-5.838916	-0.324849	2.289710
H	-4.522647	0.493155	3.167064
H	-4.538338	-1.280889	3.020121
H	-2.873426	-0.432923	1.451895
H	-4.207260	-1.106592	0.540276
H	-5.834365	1.715937	1.371824
H	-6.031515	3.781851	0.042082
H	-4.337547	4.306160	-1.722071
H	-2.465289	2.761218	-2.120472
H	-0.356152	2.032883	-1.819407
H	-1.071360	1.016891	-3.093850
H	1.404993	0.663393	-3.030485
H	0.578062	-0.831014	-2.530654
C	0.981666	-2.226243	1.825696
C	-0.390577	-2.579481	2.335429
C	-0.645905	-2.435895	3.841107
C	-0.251030	-1.085035	4.454893
H	0.847198	-0.972982	4.459013
H	-0.552867	-1.102511	5.514732
C	-0.876678	0.140006	3.768073
C	-0.159837	0.619180	2.506082
H	0.881315	0.913993	2.729836
H	-0.684147	1.484348	2.059949
H	-0.882828	0.976415	4.492958
H	-1.942944	-0.061157	3.555056
H	-0.095283	-3.244049	4.351410
H	-1.717317	-2.618935	4.034874
H	-0.742574	-3.560835	1.975679
H	-1.190919	-1.904915	1.830899
H	1.727752	-1.975721	2.589366
H	1.397683	-2.925046	1.083463

[4]9A-01

Geometry with 77 atoms:

Total energy: -3045.599294980

Cr	-0.065967	-0.695250	1.052269
P	1.730599	0.326419	-0.535891
P	-1.563454	0.346266	-0.611101
C	-0.550531	1.045331	-2.024180
C	0.840537	0.416648	-2.170112
H	-1.120216	0.951381	-2.961275
H	-0.460053	2.122074	-1.814392
H	0.773258	-0.618238	-2.539546
H	1.439792	0.990622	-2.893654
C	3.242023	-0.651951	-0.860711
C	3.693200	-0.976126	-2.151405
C	3.971841	-1.109254	0.252403
C	4.849983	-1.743797	-2.320734
H	3.155236	-0.631898	-3.036424
C	5.132642	-1.864993	0.079565
H	3.630713	-0.874026	1.263576
C	5.571809	-2.186993	-1.209210
H	5.190119	-1.991444	-3.329221
H	5.692010	-2.209278	0.952803
H	6.476528	-2.784080	-1.346439
C	2.298619	2.050912	-0.251083
C	3.618176	2.468465	-0.492467
C	1.360417	2.986512	0.226344
C	3.986645	3.798106	-0.265791
H	4.361983	1.757092	-0.857850
C	1.730456	4.316245	0.440541
H	0.330862	2.682371	0.431255
C	3.046171	4.723590	0.196772
H	5.016122	4.112153	-0.455145
H	0.990171	5.032826	0.804742
H	3.338905	5.761950	0.370242
C	-2.700350	-0.878324	-1.363008
C	-3.985251	-1.060084	-0.823314
C	-2.268882	-1.713478	-2.407403
C	-4.824426	-2.057326	-1.326746
H	-4.337611	-0.418544	-0.012709
C	-3.113488	-2.706722	-2.909325
H	-1.269702	-1.602780	-2.832963
C	-4.391421	-2.882264	-2.369275
H	-5.822893	-2.187274	-0.902265
H	-2.769605	-3.347415	-3.724962
H	-5.049769	-3.661015	-2.761729
C	-2.638270	1.751891	-0.132972
C	-3.428990	2.399247	-1.100558
C	-2.662286	2.209257	1.193808
C	-4.221254	3.490799	-0.743244
H	-3.433655	2.044325	-2.134373
C	-3.458826	3.303665	1.548332
H	-2.069678	1.706134	1.959137
C	-4.235889	3.945521	0.581178
H	-4.833447	3.987270	-1.500074
H	-3.474364	3.650333	2.584363
H	-4.859047	4.799409	0.858094
C	-1.689881	-1.366123	2.166881
C	-1.392157	-2.497328	3.162051
C	-1.053997	-3.847365	2.506809
C	0.391004	-4.003935	2.013493
C	0.927505	-2.873999	1.124919
C	0.089396	-2.418490	-0.035958
H	-2.109686	-0.492429	2.698585
H	-2.473093	-1.702454	1.465415
H	-0.578538	-2.212885	3.859643
H	-2.277755	-2.649309	3.807900
H	-1.243907	-4.661670	3.225569
H	-1.756912	-4.017768	1.672595
H	0.480780	-4.947367	1.448627
H	1.062405	-4.102509	2.884858
H	1.110610	-1.993914	1.849191
H	1.967317	-3.077397	0.823416
H	-0.878558	-2.919114	-0.150425
H	0.623786	-2.371086	-0.993766
C	1.556952	0.314346	3.075657
C	0.365030	0.930623	3.160064
H	2.370741	0.731878	2.475663
H	1.783021	-0.577640	3.668594
H	-0.419995	0.567437	3.827396
H	0.181119	1.874371	2.638051

[4]9A-02

Geometry with 77 atoms:

Total energy: -3045.599211010

Cr	-0.052909	-0.733082	1.033011
P	1.729698	0.342646	-0.536228
P	-1.552265	0.322953	-0.616459
C	-0.545654	1.022439	-2.035177
C	0.851631	0.405968	-2.175919
H	-1.112653	0.913535	-2.971805
H	-0.463705	2.101486	-1.834517
H	0.791495	-0.631100	-2.539454
H	1.447751	0.980929	-2.901354
C	3.267205	-0.601767	-0.826499
C	4.037317	-0.945852	0.301099
C	3.691919	-1.021505	-2.097872
C	5.211740	-1.686029	0.158543
H	3.717374	-0.631734	1.298708
C	4.863862	-1.773056	-2.235142
H	3.121766	-0.766062	-2.993054
C	5.625035	-2.104740	-1.111476
H	5.802980	-1.942753	1.040873
H	5.183983	-2.096338	-3.228706
H	6.540704	-2.690168	-1.223941
C	2.251289	2.081698	-0.253881
C	1.290979	2.988110	0.234745
C	3.555175	2.538016	-0.510022
C	1.624097	4.327801	0.447867
H	0.273940	2.650567	0.449378
C	3.886971	3.877324	-0.284593
H	4.315258	1.848725	-0.884391
C	2.924717	4.773660	0.190905
H	0.867566	5.021953	0.821933
H	4.904611	4.221965	-0.484424
H	3.189042	5.819631	0.364391
C	-2.710938	-0.879648	-1.370367
C	-4.003561	-1.032542	-0.841541
C	-2.287521	-1.722803	-2.411618
C	-4.860522	-2.009564	-1.354827
H	-4.347771	-0.385867	-0.031369
C	-3.150254	-2.695055	-2.923549
H	-1.281702	-1.631986	-2.827098
C	-4.437135	-2.841436	-2.395709
H	-5.865560	-2.117815	-0.939854
H	-2.814257	-3.341888	-3.737634
H	-5.110104	-3.603263	-2.796509
C	-2.606082	1.735850	-0.107822
C	-3.228357	2.550472	-1.072256
C	-2.802435	2.013181	1.254390

C	-4.018535	3.630126	-0.675028
H	-3.103474	2.342023	-2.137752
C	-3.598085	3.094267	1.648534
H	-2.344834	1.377730	2.012630
C	-4.202821	3.905265	0.685388
H	-4.496612	4.258268	-1.430623
H	-3.746035	3.299225	2.711635
H	-4.823018	4.750966	0.992437
C	-1.665961	-1.489475	2.115773
C	-1.324300	-2.623772	3.094028
C	-0.931615	-3.950570	2.423022
C	0.518913	-4.042412	1.929866
C	1.010606	-2.876603	1.062126
C	0.151812	-2.431828	-0.088257
H	-2.130819	-0.651635	2.665496
H	-2.426483	-1.845111	1.398616
H	-0.524480	-2.315898	3.797942
H	-2.204337	-2.819977	3.735580
H	-1.089325	-4.780382	3.131732
H	-1.626861	-4.138842	1.586256
H	0.645888	-4.971075	1.347942
H	1.192973	-4.130789	2.800188
H	1.165239	-2.004176	1.803719
H	2.056317	-3.034827	0.753673
H	-0.801365	-2.959857	-0.202587
H	0.679365	-2.365411	-1.048283
C	1.389757	0.355513	3.034921
C	0.188048	0.953853	3.114361
H	2.204488	0.793853	2.451455
H	1.626178	-0.532044	3.630852
H	-0.595045	0.571482	3.773048
H	-0.013954	1.897334	2.598846

C	-3.999642	3.645154	-0.697371
H	-3.120052	2.320741	-2.150753
C	-3.531513	3.156821	1.627982
H	-2.281060	1.440228	2.002736
C	-4.153191	3.949910	0.660603
H	-4.490148	4.260045	-1.455887
H	-3.655533	3.385444	2.689285
H	-4.762712	4.805135	0.962609
C	-1.693904	-1.459538	2.116271
C	-1.395867	-2.606553	3.093962
C	-1.033386	-3.941534	2.421649
C	0.420842	-4.072874	1.948516
C	0.955365	-2.919869	1.088800
C	0.124123	-2.458554	-0.077184
H	-2.127002	-0.603539	2.665337
H	-2.467579	-1.786990	1.399912
H	-0.594095	-2.325166	3.806504
H	-2.287839	-2.779480	3.725576
H	-1.224997	-4.769559	3.124062
H	-1.721803	-4.105853	1.574236
H	0.530377	-5.004355	1.367575
H	1.079920	-4.179751	2.828217
H	1.117440	-2.050729	1.830391
H	2.001065	-3.106266	0.796271
H	-0.836795	-2.969282	-0.206540
H	0.668600	-2.402126	-1.028763
C	0.291825	0.845844	3.188445
C	1.547714	0.412548	2.982772
H	-0.385524	0.333589	3.875949
H	-0.064127	1.780972	2.744619
H	2.251629	0.979952	2.367967
H	1.935875	-0.472054	3.498332

C	-4.175088	3.511935	-0.680052
H	-3.467185	2.042421	-2.090806
C	-3.326720	3.327402	1.581784
H	-1.950912	1.705924	1.947085
C	-4.129039	3.976565	0.640225
H	-4.807355	4.014558	-1.416016
H	-3.295318	3.681582	2.614923
H	-4.724880	4.844129	0.934246
C	-1.669599	-1.396047	2.161372
C	-1.383222	-2.545270	3.139729
C	-1.049210	-3.888160	2.467231
C	0.400028	-4.047881	1.986296
C	0.947206	-2.914114	1.108758
C	0.112408	-2.458138	-0.058885
H	-2.060662	-0.517301	2.707924
H	-2.470256	-1.707591	1.467825
H	-0.569612	-2.278190	3.843672
H	-2.272269	-2.700917	3.779955
H	-1.251610	-4.710950	3.172763
H	-1.745360	-4.042347	1.624223
H	0.490354	-4.988194	1.416327
H	1.062905	-4.154710	2.863138
H	1.124977	-2.036817	1.833588
H	1.988404	-3.120367	0.811563
H	-0.853440	-2.962583	-0.178028
H	0.651745	-2.414890	-1.014367
C	0.441011	0.697996	3.392489
C	1.695029	0.387395	3.025465
H	-0.137606	0.059223	4.063976
H	-0.015201	1.649099	3.098479
H	2.295416	1.067031	2.414344
H	2.186282	-0.521575	3.387529

^{4}9A-03
Geometry with 77 atoms:
Total energy: -3045.599247120

Cr	-0.063673	-0.752378	1.028234
P	1.732002	0.305058	-0.534324
P	-1.547218	0.331731	-0.625572
C	-0.529161	1.019849	-2.040418
C	0.860517	0.386085	-2.177856
H	-1.095315	0.920360	-2.978623
H	-0.433426	2.097110	-1.835695
H	0.793239	-0.649493	-2.545589
H	1.464491	0.958597	-2.898787
C	3.284128	-0.612397	-0.838401
C	4.005283	-1.059476	0.284868
C	3.777726	-0.896157	-2.123013
C	5.199284	-1.764983	0.126892
H	3.631463	-0.857440	1.291781
C	4.968621	-1.612930	-2.277403
H	3.244958	-0.560362	-3.014352
C	5.681763	-2.045520	-1.156138
H	5.751604	-2.102328	1.007294
H	5.341989	-1.829329	-3.281300
H	6.613202	-2.602864	-1.281305
C	2.229212	2.047185	-0.227117
C	1.264508	2.921326	0.308708
C	3.516622	2.535163	-0.505397
C	1.575181	4.262512	0.543697
H	0.261889	2.554946	0.543490
C	3.826721	3.876053	-0.258402
H	4.280764	1.869163	-0.912577
C	2.858941	4.741267	0.261686
H	0.814843	4.931958	0.953390
H	4.831592	4.246556	-0.475739
H	3.106206	5.788586	0.451479
C	-2.712962	-0.862348	-1.381890
C	-4.010901	-1.001230	-0.862150
C	-2.288444	-1.716285	-2.413978
C	-4.871453	-1.975368	-1.375090
H	-4.356208	-0.346315	-0.059095
C	-3.154598	-2.685642	-2.925425
H	-1.278779	-1.637033	-2.822139
C	-4.446493	-2.818378	-2.406315
H	-5.880399	-2.073011	-0.967055
H	-2.817099	-3.341237	-3.731845
H	-5.122006	-3.578378	-2.806313
C	-2.586359	1.755095	-0.119440
C	-3.223806	2.552860	-1.087873
C	-2.750402	2.062766	1.240375

^{4}9A-04
Geometry with 77 atoms:
Total energy: -3045.598675410

Cr	-0.057015	-0.740940	1.022726
P	1.730676	0.307108	-0.550600
P	-1.556910	0.331177	-0.621281
C	-0.541210	1.022544	-2.035314
C	0.840719	0.374657	-2.184663
H	-1.115349	0.941847	-2.970854
H	-0.433795	2.096171	-1.816010
H	0.758596	-0.663511	-2.540644
H	1.444105	0.932851	-2.917420
C	3.280717	-0.609323	-0.865492
C	3.657193	-1.082816	-2.133452
C	4.107514	-0.885344	0.240567
C	4.837822	-1.817469	-2.288159
H	3.043049	-0.883629	-3.013455
C	5.288758	-1.610395	0.080081
H	3.829337	-0.525883	1.234577
C	5.654562	-2.081653	-1.186042
H	5.120060	-2.181717	-3.278989
H	5.923552	-1.812965	0.946061
H	6.576301	-2.654635	-1.312131
C	2.212980	2.056078	-0.267176
C	3.455532	2.581381	-0.658441
C	1.270666	2.902636	0.346353
C	3.743711	3.932398	-0.443641
H	4.201349	1.936279	-1.128684
C	1.558341	4.254372	0.549018
H	0.302071	2.508778	0.666033
C	2.797433	4.770368	0.155652
H	4.713538	4.333082	-0.748878
H	0.814760	4.902655	1.019050
H	3.027326	5.826030	0.319285
C	-2.715641	-0.875845	-1.365981
C	-3.998809	-1.041344	-0.816719
C	-2.302091	-1.716222	-2.413440
C	-4.854422	-2.027190	-1.314783
H	-4.336930	-0.395977	-0.003049
C	-3.163163	-2.698145	-2.909687
H	-1.304632	-1.617921	-2.846044
C	-4.439545	-2.856978	-2.360845
H	-5.851446	-2.144563	-0.883308
H	-2.833584	-3.342958	-3.727970
H	-5.110895	-3.626669	-2.749123
C	-2.601456	1.749348	-0.118918
C	-3.417193	2.403595	-1.060301
C	-2.565879	2.215915	1.203976

^{4}9A-05
Geometry with 77 atoms:
Total energy: -3045.599083050

Cr	-0.061526	-0.733049	1.045898
P	1.739640	0.354186	-0.518317
P	-1.560123	0.350077	-0.589370
C	-0.548011	1.061054	-1.998377
C	0.841679	0.431217	-2.149922
H	-1.118562	0.972473	-2.935281
H	-0.456709	2.136325	-1.782268
H	0.765666	-0.603836	-2.515120
H	1.441354	0.998778	-2.878411
C	3.258059	-0.616474	-0.838034
C	3.591759	-1.144948	-2.096152
C	4.103134	-0.880114	0.257109
C	4.742878	-1.925242	-2.250296
H	2.967489	-0.953436	-2.970356
C	5.255455	-1.650557	0.097679
H	3.866984	-0.470671	1.242749
C	5.575022	-2.180295	-1.157759
H	4.990164	-2.331830	-3.233943
H	5.903966	-1.841733	0.956014
H	6.473415	-2.789316	-1.283213
C	2.295749	2.088402	-0.260404
C	3.603301	2.518666	-0.542067
C	1.357302	3.021740	0.221144
C	3.960972	3.855881	-0.345626
H	4.347084	1.811350	-0.915059
C	1.716129	4.359357	0.404717
H	0.335333	2.710795	0.450961
C	3.020931	4.777851	0.124890
H	4.981702	4.178631	-0.565341
H	0.975370	5.073206	0.773272
H	3.305351	5.822098	0.275339
C	-2.715612	-0.847063	-1.358059
C	-3.998567	-1.024355	-0.812407
C	-2.303365	-1.663511	-2.424727
C	-4.855320	-1.997763	-1.332510
H	-4.335939	-0.397217	0.015739
C	-3.165601	-2.632817	-2.943392
H	-1.306212	-1.556267	-2.856104
C	-4.441902	-2.803241	-2.397953
H	-5.852317	-2.123994	-0.903463
H	-2.837101	-3.258347	-3.776969
H	-5.114397	-3.562635	-2.804126
C	-2.619294	1.758445	-0.085356
C	-3.386190	2.449203	-1.042014
C	-2.656486	2.171275	1.255062

C	-4.166298	3.540934	-0.659455
H	-3.381535	2.128531	-2.086906
C	-3.440945	3.265674	1.635404
H	-2.081596	1.632070	2.008434
C	-4.193189	3.951829	0.679126
H	-4.759607	4.072058	-1.407757
H	-3.466145	3.578037	2.682128
H	-4.806642	4.806299	0.975301
C	-1.672239	-1.456870	2.143675
C	-1.353726	-2.619619	3.094882
C	-1.000009	-3.941326	2.391908
C	0.445122	-4.061556	1.887799
C	0.959285	-2.898305	1.028926
C	0.099742	-2.416742	-0.103860
H	-2.084349	-0.603309	2.712870
H	-2.464772	-1.770545	1.442305
H	-0.541247	-2.347204	3.797709
H	-2.233962	-2.806501	3.738964
H	-1.175416	-4.782057	3.083381
H	-1.704782	-4.093112	1.555653
H	0.545778	-4.986665	1.295145
H	1.122307	-4.175594	2.752666
H	1.143593	-2.040183	1.779851
H	1.998210	-3.078107	0.707967
H	-0.864723	-2.923360	-0.219536
H	0.618847	-2.336207	-1.067242
C	0.341417	0.926324	3.118863
C	1.365395	0.062001	3.228388
H	-0.584065	0.781449	3.681202
H	0.442175	1.851009	2.544007
H	2.324898	0.251512	2.738974
H	1.304810	-0.817591	3.877010

C	-4.394948	2.650137	-1.907018
H	-2.384606	2.157487	-2.479969
C	-5.406326	1.264631	-0.200928
H	-4.186619	-0.330845	0.579709
C	-5.487591	2.338962	-1.093760
H	-4.454448	3.483569	-2.611284
H	-6.258483	1.013716	0.435226
H	-6.403759	2.931002	-1.156680
C	-1.802382	0.954410	2.395316
C	-1.571034	1.402600	3.843814
C	-0.921186	0.354779	4.759415
C	0.593102	0.180592	4.584360
C	1.077907	-0.084230	3.151641
C	0.345545	-1.115541	2.340812
H	-2.340143	1.741257	1.834547
H	-2.453667	0.061703	2.387006
H	-0.968775	2.330949	3.878413
H	-2.545615	1.681121	4.288318
H	-1.100780	0.628278	5.812392
H	-1.432944	-0.612555	4.613924
H	0.935253	-0.661950	5.209022
H	1.109324	1.078182	4.968132
H	1.028675	0.948623	2.625340
H	2.168853	-0.242457	3.134513
H	-0.499921	-1.594669	2.847762
H	0.996431	-1.851068	1.855359
C	0.369822	3.154437	1.222744
C	-0.232262	2.958534	0.036455
H	1.460559	3.176275	1.304993
H	-0.203249	3.384891	2.124576
H	-1.319108	3.020561	-0.070490
H	0.357215	2.818174	-0.874614

C	-3.116939	3.855186	0.586288
H	-1.571125	3.254062	-0.777195
C	-4.401256	2.084048	1.617063
H	-3.863639	0.071649	1.067542
C	-4.136582	3.448400	1.449906
H	-2.913924	4.918687	0.438019
H	-5.205264	1.757963	2.281241
H	-4.730923	4.192371	1.985730
C	-1.599798	-1.760025	1.987997
C	-1.197245	-2.700467	3.132824
C	-0.472229	-3.983271	2.693565
C	1.017758	-3.823921	2.358802
C	1.371802	-2.685404	1.392220
C	0.577901	-2.562158	0.119014
H	-2.252541	-0.958630	2.375213
H	-2.196462	-2.315182	1.241966
H	-0.577175	-2.167720	3.881741
H	-2.107889	-3.002786	3.684280
H	-0.549979	-4.739115	3.492505
H	-1.009436	-4.411613	1.829038
H	1.394057	-4.764801	1.922529
H	1.584758	-3.670481	3.293918
H	1.265430	-1.727669	2.028286
H	2.456512	-2.657524	1.201917
H	-0.219106	-3.306787	0.013953
H	1.183704	-2.510746	-0.795617
C	-0.393978	1.056602	2.961864
C	0.903182	0.709862	3.033799
H	-0.743683	1.879762	2.331452
H	-1.147858	0.573160	3.587562
H	1.245420	-0.057030	3.736054
H	1.674224	1.244022	2.470834

^{4}9A-06
Geometry with 77 atoms:
Total energy: -3045.597799740

Cr	-0.150046	0.506745	1.220421
P	1.731133	-0.062239	-0.631842
P	-1.600106	-0.158884	-0.704718
C	-0.586695	0.097984	-2.246482
C	0.756893	-0.628032	-2.120664
H	-1.153724	-0.267370	-3.117134
H	-0.432773	1.179779	-2.380053
H	0.595393	-1.708457	-1.983252
H	1.360467	-0.524979	-3.034944
C	2.947516	-1.423979	-0.402848
C	2.450221	-2.722572	-0.175429
C	4.336866	-1.219327	-0.408332
C	3.325117	-3.789550	0.037239
H	1.373852	-2.913757	-0.172262
C	5.208258	-2.291009	-0.188436
H	4.750519	-0.226790	-0.594278
C	4.707387	-3.575918	0.035747
H	2.923562	-4.791854	0.205444
H	6.287080	-2.117240	-0.200184
H	5.391843	-4.410546	0.205405
C	2.695442	1.399772	-1.177119
C	3.458584	2.072514	-0.202710
C	2.656610	1.915394	-2.482647
C	4.181662	3.220305	-0.532634
H	3.497277	1.689739	0.821445
C	3.368487	3.075540	-2.806137
H	2.074442	1.421200	-3.262544
C	4.133309	3.727869	-1.835805
H	4.779636	3.723433	0.231113
H	3.328129	3.466122	-3.825876
H	4.691597	4.631061	-2.093346
C	-2.128514	-1.909630	-0.850758
C	-1.622459	-2.881149	0.026398
C	-3.010892	-2.295458	-1.876828
C	-1.986880	-4.223583	-0.124366
H	-0.950216	-2.588603	0.831722
C	-3.372295	-3.635507	-2.021902
H	-3.425874	-1.548073	-2.557810
C	-2.859698	-4.601654	-1.147235
H	-1.590709	-4.972258	0.565947
H	-4.060206	-3.927925	-2.818927
H	-3.147558	-5.649535	-1.262265
C	-3.132301	0.814881	-0.934539
C	-3.220686	1.893948	-1.830166
C	-4.236782	0.507978	-0.118214

^{4}9A-07
Geometry with 77 atoms:
Total energy: -3045.597897370

Cr	-0.046234	-0.820466	0.988033
P	1.710901	0.345820	-0.560937
P	-1.581232	0.207391	-0.680292
C	-0.565120	0.998063	-2.038588
C	0.804533	0.323952	-2.187776
H	-1.135234	0.946174	-2.977988
H	-0.431719	2.062781	-1.799798
H	0.690711	-0.731812	-2.481018
H	1.401134	0.829490	-2.963020
C	3.290207	-0.528778	-0.841746
C	3.609709	-1.176674	-2.045789
C	4.196854	-0.595348	0.233970
C	4.815749	-1.875548	-2.170156
H	2.929224	-1.143143	-2.898689
C	5.402550	-1.285072	0.101995
H	3.964500	-0.097199	1.179906
C	5.712809	-1.930431	-1.100917
H	5.054380	-2.376016	-3.111791
H	6.101456	-1.322414	0.941191
H	6.654641	-2.474802	-1.203104
C	2.163899	2.114478	-0.360172
C	3.368055	2.657502	-0.839752
C	1.236548	2.958672	0.275231
C	3.631892	4.021199	-0.684684
H	4.102976	2.015702	-1.330882
C	1.498110	4.323356	0.419700
H	0.299176	2.547961	0.654374
C	2.699597	4.855696	-0.057960
H	4.572101	4.435240	-1.057240
H	0.765600	4.967427	0.912665
H	2.912426	5.920877	0.061159
C	-2.776041	-0.860230	-1.573589
C	-2.491285	-2.223533	-1.750898
C	-3.945614	-0.318636	-2.137037
C	-3.362885	-3.034357	-2.484054
H	-1.591164	-2.653327	-1.313313
C	-4.814072	-1.134412	-2.864880
H	-4.185620	0.738613	-2.003182
C	-4.524895	-2.492496	-3.039578
H	-3.134200	-4.094889	-2.614424
H	-5.722427	-0.707125	-3.296710
H	-5.208793	-3.128371	-3.607124
C	-2.605164	1.534565	0.069141
C	-2.354178	2.905439	-0.102942
C	-3.642155	1.133120	0.934415

^{4}9A-08
Geometry with 77 atoms:
Total energy: -3045.596768370

Cr	-0.092301	-0.428285	1.236712
P	1.732824	0.289398	-0.591181
P	-1.634222	0.154776	-0.641695
C	-0.604462	0.996111	-1.945148
C	0.720770	0.249888	-2.146999
H	-1.180832	1.047755	-2.881594
H	-0.415950	2.028241	-1.613436
H	0.533847	-0.811880	-2.376344
H	1.282025	0.664525	-2.997916
C	3.162024	-0.820820	-0.906342
C	3.404650	-1.425556	-2.150947
C	4.036023	-1.088258	0.163412
C	4.499342	-2.280034	-2.317284
H	2.752488	-1.236070	-3.004988
C	5.133624	-1.933362	-0.009340
H	3.864074	-0.629788	1.140527
C	5.364911	-2.535294	-1.250607
H	4.677205	-2.744203	-3.290528
H	5.806621	-2.127575	0.829283
H	6.219685	-3.202290	-1.385587
C	2.462433	1.982468	-0.534589
C	2.306504	2.934819	-1.555673
C	3.182641	2.341822	0.619837
C	2.853778	4.215244	-1.419496
H	1.764908	2.694576	-2.472211
C	3.738867	3.615558	0.748284
H	3.320974	1.616876	1.425995
C	3.569788	4.559234	-0.270355
H	2.723191	4.944797	-2.222684
H	4.301064	3.874109	1.648922
H	3.996382	5.559892	-0.168128
C	-2.477742	-1.178040	-1.582826
C	-1.909764	-2.461177	-1.640066
C	-3.648759	-0.909315	-2.315454
C	-2.500738	-3.459265	-2.421055
H	-1.010203	-2.686700	-1.069691
C	-4.237420	-1.911793	-3.088745
H	-4.107836	0.081033	-2.279975
C	-3.665004	-3.187526	-3.143986
H	-2.051436	-4.454678	-2.456289
H	-5.149301	-1.694892	-3.650574
H	-4.130119	-3.970116	-3.748436
C	-2.963501	1.336791	-0.204395
C	-4.017290	0.864807	0.601563
C	-2.944172	2.689594	-0.582187

C	-5.028049	1.731041	1.020163
H	-4.051633	-0.185163	0.899280
C	-3.958725	3.553914	-0.157348
H	-2.146358	3.087073	-1.211455
C	-4.999311	3.078926	0.644919
H	-5.841564	1.351228	1.642879
H	-3.934771	4.603295	-0.460853
H	-5.790258	3.756654	0.974947
C	-1.662826	-0.907383	2.500137
C	-1.343493	-1.563340	3.849970
C	-0.711056	-2.960435	3.760622
C	0.787875	-2.974820	3.433390
C	1.209431	-2.159140	2.203524
C	0.442084	-2.366370	0.926943
H	-2.189433	0.050975	2.662311
H	-2.351804	-1.559299	1.932423
H	-0.691128	-0.910076	4.462142
H	-2.280916	-1.652611	4.431363
H	-0.845017	-3.486518	4.720255
H	-1.267459	-3.556231	3.016120
H	1.116863	-4.015184	3.270561
H	1.353071	-2.604922	4.307024
H	1.131826	-1.055130	2.548836
H	2.296240	-2.233580	2.042850
H	-0.396047	-3.068527	1.003071
H	1.068976	-2.585884	0.052265
C	0.424987	1.612733	2.870789
C	-0.283485	2.187619	1.882296
H	1.518910	1.624520	2.870531
H	-0.065538	1.193788	3.754078
H	-1.373677	2.254839	1.926364
H	0.215497	2.681513	1.042663

C	-4.128964	3.097167	-1.569116
H	-2.137240	2.552616	-2.160356
C	-5.293584	1.545205	-0.124123
H	-4.214206	-0.233711	0.431701
C	-5.269188	2.746012	-0.842083
H	-4.106846	4.029696	-2.138220
H	-6.183688	1.261746	0.442671
H	-6.140475	3.405403	-0.837368
C	-1.966768	0.299272	2.501965
C	-1.831951	0.314201	4.029785
C	-1.336841	-0.998923	4.653152
C	0.172429	-1.246730	4.538956
C	0.768907	-1.111069	3.130679
C	0.067044	-1.807819	1.998244
H	-2.428380	1.240804	2.154546
H	-2.650288	-0.516187	2.205444
H	-1.176080	1.142513	4.361853
H	-2.821691	0.544244	4.468133
H	-1.593069	-1.015263	5.725440
H	-1.894652	-1.838551	4.202937
H	0.402523	-2.263564	4.899774
H	0.706439	-0.552275	5.211034
H	0.811921	0.030794	2.937840
H	1.849745	-1.327661	3.153967
H	-0.847859	-2.344865	2.271985
H	0.713181	-2.426139	1.363748
C	0.351447	2.593772	2.003274
C	-0.317257	2.741466	0.844663
H	1.444982	2.564427	2.024938
H	-0.168612	2.590573	2.965430
H	-1.404012	2.860127	0.818188
H	0.217623	2.838064	-0.105404

C	-5.089314	2.385152	-1.054572
H	-4.497605	0.339058	-1.378524
C	-3.335288	3.929226	-0.430757
H	-1.358246	3.103328	-0.251248
C	-4.681812	3.677829	-0.716575
H	-6.138360	2.183538	-1.284652
H	-3.007682	4.939010	-0.171511
H	-5.411124	4.490580	-0.677778
C	-1.990490	0.026010	2.460739
C	-1.962912	-0.565759	3.875887
C	-1.810470	-2.093561	3.937153
C	-0.379259	-2.612181	3.745731
C	0.356273	-2.100602	2.498785
C	-0.368935	-2.173833	1.185871
H	-2.182383	1.113745	2.505854
H	-2.842572	-0.407759	1.909767
H	-1.164695	-0.100540	4.485483
H	-2.904796	-0.296876	4.390712
H	-2.165112	-2.458982	4.915056
H	-2.482253	-2.550408	3.189249
H	-0.394665	-3.714128	3.693707
H	0.221295	-2.352900	4.635271
H	0.624501	-0.999239	2.744338
H	1.371117	-2.527846	2.453177
H	-1.385971	-2.576183	1.232927
H	0.184600	-2.619640	0.349809
C	0.857705	1.678457	2.917668
C	0.288968	2.424170	1.954154
H	1.908244	1.379154	2.857330
H	0.316739	1.415593	3.831113
H	-0.737100	2.788744	2.049922
H	0.861338	2.758506	1.083831

^{4}9A-09
Geometry with 77 atoms:
Total energy: -3045.596099180

Cr	-0.248264	0.094946	1.357145
P	1.796837	0.023565	-0.464812
P	-1.581303	-0.066714	-0.754022
C	-0.447870	0.440104	-2.138762
C	0.883340	-0.315432	-2.054210
H	-0.951290	0.253477	-3.100452
H	-0.288952	1.524812	-2.050013
H	0.712809	-1.404635	-2.068796
H	1.523995	-0.088789	-2.920385
C	3.205584	-1.156765	-0.555830
C	4.102620	-1.095225	-1.638279
C	3.405638	-2.119597	0.445016
C	5.167899	-1.992322	-1.722528
H	3.979017	-0.332767	-2.411766
C	4.476833	-3.015959	0.359601
H	2.731143	-2.174726	1.299476
C	5.355660	-2.955956	-0.724112
H	5.859289	-1.935872	-2.566972
H	4.623580	-3.760580	1.145777
H	6.192658	-3.655473	-0.790024
C	2.634477	1.643047	-0.728791
C	2.463213	2.448902	-1.866217
C	3.474046	2.098896	0.305370
C	3.107985	3.688069	-1.959601
H	1.836109	2.123341	-2.698024
C	4.122559	3.330606	0.205820
H	3.635319	1.475980	1.190569
C	3.935055	4.132663	-0.925810
H	2.965378	4.304000	-2.851017
H	4.776855	3.666565	1.014025
H	4.438060	5.099513	-1.002529
C	-2.210628	-1.699658	-1.312134
C	-3.230542	-1.775851	-2.278748
C	-1.624407	-2.882975	-0.835652
C	-3.654104	-3.018034	-2.754407
H	-3.701517	-0.865349	-2.656262
C	-2.049287	-4.124431	-1.319450
H	-0.840328	-2.838350	-0.081807
C	-3.064406	-4.194038	-2.276669
H	-4.450042	-3.067990	-3.501558
H	-1.586539	-5.038871	-0.940560
H	-3.399844	-5.164677	-2.650117
C	-3.027892	1.050269	-0.857316
C	-3.011685	2.255521	-1.579034
C	-4.180974	0.703301	-0.128126

^{4}9A-10
Geometry with 77 atoms:
Total energy: -3045.595946660

Cr	-0.284083	-0.149904	1.293143
P	1.829753	0.014533	-0.444972
P	-1.535846	0.261935	-0.808559
C	-0.334105	0.820220	-2.111318
C	0.974053	0.021052	-2.102360
H	-0.819209	0.793996	-3.099530
H	-0.151324	1.882109	-1.889183
H	0.786212	-1.041682	-2.324121
H	1.667233	0.386077	-2.877030
C	3.177050	-1.208367	-0.721965
C	4.276830	-0.884439	-1.537984
C	3.101697	-2.488834	-0.151675
C	5.276717	-1.828025	-1.779041
H	4.359343	0.112012	-1.978879
C	4.105423	-3.432017	-0.395580
H	2.258542	-2.758711	0.483473
C	5.193026	-3.103408	-1.208372
H	6.127367	-1.565634	-2.412959
H	4.035719	-4.425277	0.054494
H	5.978945	-3.839099	-1.396116
C	2.750980	1.605647	-0.361036
C	3.652421	1.768710	0.708626
C	2.570731	2.668800	-1.260828
C	4.347793	2.966304	0.878128
H	3.828092	0.943482	1.405204
C	3.264380	3.872177	-1.084190
H	1.898575	2.576700	-2.115171
C	4.149509	4.025763	-0.014991
H	5.048939	3.073310	1.709376
H	3.114362	4.689582	-1.793827
H	4.689768	4.965762	0.120027
C	-2.345301	-1.246113	-1.468788
C	-3.252230	-1.937948	-0.643404
C	-2.081050	-1.746009	-2.754714
C	-3.884153	-3.095961	-1.098268
H	-3.473862	-1.567149	0.358445
C	-2.707023	-2.914246	-3.201890
H	-1.389426	-1.235936	-3.426730
C	-3.608994	-3.590650	-2.377623
H	-4.591239	-3.616189	-0.447711
H	-2.488701	-3.292102	-4.203633
H	-4.098768	-4.501300	-2.730773
C	-2.809823	1.583991	-0.813085
C	-4.160677	1.340338	-1.105560
C	-2.406131	2.888771	-0.473445

^{4}9A-11
Geometry with 77 atoms:
Total energy: -3045.595498210

Cr	-0.163361	-0.225329	1.258949
P	1.772346	0.199726	-0.541695
P	-1.584821	0.282629	-0.704121
C	-0.476765	1.056434	-1.975712
C	0.817949	0.247478	-2.134996
H	-1.004417	1.171130	-2.934290
H	-0.254857	2.073865	-1.621627
H	0.588226	-0.798944	-2.390840
H	1.434199	0.648966	-2.953527
C	3.079970	-1.064365	-0.796233
C	3.383863	-1.611205	-2.054346
C	3.803179	-1.500386	0.328629
C	4.388824	-2.575346	-2.178801
H	2.847895	-1.291962	-2.950089
C	4.814437	-2.454455	0.199178
H	3.574627	-1.094016	1.316647
C	5.106444	-2.997189	-1.056021
H	4.614178	-2.995106	-3.162236
H	5.369699	-2.780376	1.082099
H	5.892091	-3.749724	-1.158393
C	2.688999	1.799801	-0.479509
C	2.567648	2.802110	-1.456112
C	3.512055	2.040530	0.637231
C	3.250684	4.015456	-1.316100
H	1.948506	2.652124	-2.341877
C	4.200424	3.247535	0.769358
H	3.628309	1.276089	1.410601
C	4.067022	4.241948	-0.205700
H	3.147051	4.783934	-2.086263
H	4.840792	3.413885	1.638939
H	4.600386	5.189582	-0.099962
C	-2.333841	-1.176745	-1.531297
C	-2.933241	-2.174253	-0.741596
C	-2.347669	-1.315873	-2.929639
C	-3.540482	-3.281364	-1.338243
H	-2.929885	-2.085295	0.345026
C	-2.944466	-2.432036	-3.522294
H	-1.900147	-0.557765	-3.573916
C	-3.543207	-3.415329	-2.729748
H	-4.007407	-4.044760	-0.711367
H	-2.944555	-2.529363	-4.610624
H	-4.011619	-4.285161	-3.196526
C	-2.962772	1.474800	-0.464464
C	-4.238236	1.007069	-0.102940
C	-2.745234	2.862015	-0.549291

C	-5.272307	1.907977	0.162281
H	-4.436779	-0.063799	-0.036165
C	-3.784195	3.758773	-0.286295
H	-1.766603	3.261803	-0.820473
C	-5.049551	3.284954	0.071592
H	-6.259097	1.528264	0.437834
H	-3.601247	4.833335	-0.363822
H	-5.860687	3.987484	0.277144
C	-1.794675	-0.381956	2.532298
C	-1.539970	-1.059804	3.885340
C	-1.203181	-2.557048	3.796402
C	0.257500	-2.881402	3.455371
C	0.840657	-2.179946	2.221200
C	0.042854	-2.221611	0.945036
H	-2.145901	0.656052	2.679929
H	-2.617927	-0.909394	2.018945
H	-0.736891	-0.539837	4.444281
H	-2.442297	-0.949340	4.516310
H	-1.430514	-3.043553	4.759321
H	-1.877478	-3.029751	3.060451
H	0.358526	-3.968524	3.296342
H	0.892739	-2.637013	4.324999
H	1.025488	-1.085382	2.544869
H	1.882141	-2.499524	2.062526
H	-0.895984	-2.781457	1.005249
H	0.613450	-2.515457	0.053443
C	0.603265	1.837292	2.707972
C	-0.070594	2.409145	1.693648
H	1.692774	1.743564	2.680762
H	0.097962	1.528786	3.628259
H	-1.148567	2.584102	1.745753
H	0.459280	2.797095	0.817533

C	-5.173455	2.411918	-0.409987
H	-4.596458	0.410416	-0.961358
C	-3.381855	3.929056	0.170932
H	-1.389745	3.123954	0.094892
C	-4.747280	3.679367	-0.005758
H	-6.237861	2.211923	-0.555347
H	-3.039549	4.919063	0.482335
H	-5.476586	4.473877	0.169359
C	-1.775318	-0.349670	2.535334
C	-1.617971	-1.171516	3.820778
C	-1.436957	-2.680951	3.593643
C	-0.012102	-3.115369	3.226712
C	0.642312	-2.379574	2.049579
C	-0.136038	-2.255957	0.771949
H	-1.975767	0.710118	2.779372
H	-2.669628	-0.706055	1.996229
H	-0.775458	-0.794804	4.433165
H	-2.515097	-1.024251	4.451608
H	-1.722556	-3.228741	4.506851
H	-2.146349	-3.011985	2.814672
H	-0.011258	-4.191815	2.984753
H	0.637717	-2.997958	4.111810
H	0.908432	-1.326157	2.454603
H	1.656427	-2.771220	1.876343
H	-1.128701	-2.717949	0.777969
H	0.419773	-2.521843	-0.137723
C	1.014245	1.421623	2.936031
C	0.348299	2.238160	2.100039
H	2.073112	1.192131	2.779184
H	0.547889	1.030282	3.845285
H	-0.684906	2.534786	2.297803
H	0.847504	2.697482	1.241257

C	-2.559792	3.981419	1.296712
H	-1.005831	2.489031	1.377267
C	-4.340513	3.575832	-0.293027
H	-4.186009	1.775126	-1.469941
C	-3.762086	4.373548	0.699435
H	-2.101186	4.602135	2.070273
H	-5.276809	3.882770	-0.765490
H	-4.248683	5.302217	1.007317
C	-1.911608	-1.287404	2.108419
C	-1.764686	-2.419668	3.134401
C	-1.418519	-3.785164	2.520921
C	0.053676	-3.977152	2.135769
C	0.681376	-2.868521	1.280032
C	-0.054417	-2.408710	0.047599
H	-2.361570	-0.394362	2.578658
H	-2.618895	-1.619056	1.331323
H	-1.018739	-2.169911	3.914111
H	-2.720301	-2.528485	3.681671
H	-1.680460	-4.585951	3.232280
H	-2.062940	-3.948071	1.639314
H	0.163293	-4.925418	1.582570
H	0.657347	-4.085850	3.054260
H	0.838862	-1.982413	2.009244
H	1.729210	-3.115381	1.053156
H	-1.030276	-2.878556	-0.124342
H	0.549939	-2.423375	-0.869672
C	1.121935	0.996027	2.787700
C	-0.020533	0.698349	3.428776
H	2.029162	0.399880	2.927264
H	1.223434	1.893743	2.172026
H	-0.902692	1.339659	3.356187
H	-0.094815	-0.155105	4.107694

^{4}9A-12

Geometry with 77 atoms:

Total energy: -3045.596109240

Cr	-0.155978	-0.277633	1.236700
P	1.762677	0.184494	-0.570980
P	-1.594140	0.336444	-0.692390
C	-0.500958	1.047416	-2.017366
C	0.817457	0.277878	-2.170411
H	-1.050321	1.102233	-2.969470
H	-0.320051	2.088802	-1.713022
H	0.621574	-0.765477	-2.463386
H	1.438631	0.725428	-2.961885
C	3.048720	-1.095025	-0.852583
C	3.666656	-1.669842	0.271892
C	3.445475	-1.511255	-2.135066
C	4.664261	-2.636119	0.120450
H	3.367905	-1.362057	1.276455
C	4.435348	-2.486680	-2.283346
H	2.993093	-1.078486	-3.029296
C	5.046749	-3.049735	-1.158884
H	5.137700	-3.071583	1.003730
H	4.733401	-2.804658	-3.285479
H	5.821032	-3.811236	-1.279894
C	2.715250	1.760521	-0.475073
C	2.441973	2.873610	-1.287527
C	3.709232	1.873287	0.514906
C	3.142653	4.071718	-1.107845
H	1.691079	2.824552	-2.077581
C	4.410869	3.067465	0.687263
H	3.954954	1.015838	1.146819
C	4.125019	4.173720	-0.120289
H	2.920183	4.926705	-1.751139
H	5.186073	3.133535	1.454624
H	4.671194	5.109922	0.016906
C	-2.446015	-1.100343	-1.452587
C	-2.289128	-1.445899	-2.805035
C	-3.271102	-1.898890	-0.638248
C	-2.943264	-2.565764	-3.329215
H	-1.660968	-0.850802	-3.469376
C	-3.931538	-3.008173	-1.167886
H	-3.401609	-1.652112	0.416232
C	-3.766072	-3.347206	-2.514990
H	-2.809312	-2.823195	-4.382666
H	-4.573657	-3.613169	-0.523289
H	-4.277940	-4.219694	-2.928072
C	-2.873824	1.633025	-0.457455
C	-4.244567	1.391111	-0.637492
C	-2.451818	2.911983	-0.048051

^{4}9A-13

Geometry with 77 atoms:

Total energy: -3045.592831160

Cr	-0.201872	-0.661567	1.082571
P	1.744940	0.225636	-0.517545
P	-1.598722	0.482290	-0.600625
C	-0.505551	1.131100	-1.966610
C	0.817551	0.370200	-2.122251
H	-1.072630	1.146996	-2.910454
H	-0.323992	2.180856	-1.693152
H	0.643264	-0.666854	-2.446714
H	1.444772	0.848553	-2.890288
C	3.103222	-0.964902	-0.861242
C	3.739342	-1.580012	0.231667
C	3.540344	-1.267984	-2.161952
C	4.794735	-2.473188	0.031066
H	3.407272	-1.364384	1.250397
C	4.587645	-2.172132	-2.360216
H	3.076644	-0.801025	-3.032819
C	5.217111	-2.774800	-1.266975
H	5.281806	-2.940805	0.890149
H	4.916457	-2.401796	-3.376746
H	6.036810	-3.479398	-1.426751
C	2.635102	1.833065	-0.326237
C	2.385218	2.952932	-1.137169
C	3.588298	1.947213	0.703787
C	3.064315	4.156427	-0.916206
H	1.670038	2.907353	-1.959295
C	4.270705	3.145640	0.916153
H	3.813429	1.090432	1.342965
C	4.006508	4.257695	0.109219
H	2.856534	5.016096	-1.558094
H	5.013438	3.210556	1.715100
H	4.537610	5.197587	0.277505
C	-2.800880	-0.647517	-1.390358
C	-2.473991	-1.339884	-2.568734
C	-4.027715	-0.917123	-0.755705
C	-3.360331	-2.278692	-3.104276
H	-1.527096	-1.160380	-3.081367
C	-4.911222	-1.852804	-1.298047
H	-4.302112	-0.390575	0.160630
C	-4.579197	-2.537478	-2.471319
H	-3.095103	-2.809302	-4.021912
H	-5.863675	-2.047118	-0.799019
H	-5.271057	-3.270805	-2.892481
C	-2.523794	1.979563	-0.085970
C	-1.945834	2.788857	0.908091
C	-3.725210	2.385285	-0.690447

^{4}9A-14

Geometry with 77 atoms:

Total energy: -3045.594721370

Cr	-0.088625	-0.422934	1.202362
P	1.715201	0.335667	-0.527657
P	-1.681247	0.305365	-0.578578
C	-0.648091	1.091261	-1.908507
C	0.721191	0.417504	-2.098965
H	-1.203287	1.108909	-2.858843
H	-0.526964	2.139540	-1.595117
H	0.606447	-0.629599	-2.419920
H	1.289493	0.931645	-2.889661
C	3.101804	-0.805234	-0.895408
C	3.652484	-1.545586	0.163553
C	3.653464	-0.931880	-2.181694
C	4.735881	-2.400289	-0.057141
H	3.231398	-1.457737	1.168012
C	4.729152	-1.795377	-2.401529
H	3.255436	-0.354165	-3.018648
C	5.272034	-2.529504	-1.341266
H	5.155164	-2.971908	0.774297
H	5.149187	-1.891732	-3.405724
H	6.114278	-3.202955	-1.517567
C	2.537194	1.975965	-0.374548
C	3.518983	2.121367	0.623492
C	2.202566	3.088406	-1.163666
C	4.147877	3.350355	0.828170
H	3.811755	1.261644	1.233354
C	2.830061	4.321145	-0.951040
H	1.461514	3.011086	-1.961051
C	3.799914	4.456414	0.044800
H	4.914953	3.444370	1.600791
H	2.560891	5.177514	-1.574337
H	4.289447	5.419604	0.207133
C	-2.597663	-1.070521	-1.378474
C	-2.291519	-1.546485	-2.662270
C	-3.604483	-1.708582	-0.631777
C	-2.986185	-2.639852	-3.191072
H	-1.515056	-1.078122	-3.269304
C	-4.297924	-2.794996	-1.165489
H	-3.852868	-1.355795	0.372054
C	-3.988279	-3.265581	-2.446634
H	-2.740245	-3.000822	-4.192733
H	-5.082306	-3.278085	-0.577904
H	-4.528708	-4.119154	-2.862729
C	-2.983022	1.537449	-0.186747
C	-3.378917	2.526350	-1.103468
C	-3.630684	1.455976	1.058639

C	-4.399601	3.421891	-0.772601
H	-2.905020	2.605642	-2.084018
C	-4.657077	2.347514	1.380542
H	-3.328759	0.694958	1.780806
C	-5.040189	3.334451	0.467184
H	-4.699161	4.188613	-1.491191
H	-5.155366	2.272878	2.350069
H	-5.839362	4.035051	0.720727
C	-1.297362	-0.942717	2.761440
C	0.001483	-1.393644	3.376904
C	0.197639	-2.890197	3.649139
C	-0.075299	-3.824527	2.464399
C	0.647190	-3.441389	1.164914
C	-0.028741	-2.324319	0.363320
H	-1.772016	-0.097066	3.277362
H	-2.021015	-1.742280	2.559055
H	0.897647	-1.105370	2.691785
H	0.264921	-0.812122	4.274830
H	1.233817	-3.045062	3.998401
H	-0.457394	-3.163767	4.493649
H	-1.159761	-3.881881	2.265964
H	0.225295	-4.841068	2.767519
H	1.702233	-3.195771	1.385368
H	0.694131	-4.340692	0.521970
H	-1.080474	-2.597829	0.182693
H	0.448765	-2.229710	-0.628346
C	0.620898	1.804280	2.750299
C	-0.234328	2.310550	1.849224
H	0.276131	1.455585	3.727488
H	1.700063	1.796152	2.569742
H	0.124998	2.735407	0.906540
H	-1.305237	2.387840	2.051986

C	-3.254699	4.246670	-0.442255
H	-2.867888	2.729548	-1.925615
C	-2.460485	3.783439	1.799001
H	-1.454691	1.899948	2.082475
C	-3.112300	4.628445	0.897351
H	-3.770110	4.903112	-1.147476
H	-2.356905	4.072965	2.847481
H	-3.516321	5.584789	1.238245
C	-1.723803	-0.941539	2.293823
C	-1.941927	-2.300157	2.965977
C	-2.780721	-3.283304	2.136327
C	-2.345953	-3.477744	0.675423
C	-0.837899	-3.735029	0.467556
C	-0.050755	-2.535336	-0.057338
H	-1.442285	-0.175251	3.050049
H	-2.663889	-0.590039	1.834847
H	-0.973168	-2.769933	3.216913
H	-2.446774	-2.168216	3.941969
H	-2.775848	-4.261352	2.649961
H	-3.832154	-2.944137	2.139764
H	-2.639773	-2.596588	0.084774
H	-2.929129	-4.315533	0.259554
H	-0.386176	-4.114816	1.401380
H	-0.707584	-4.561026	-0.257764
H	-0.440087	-2.242713	-1.048377
H	1.020579	-2.781592	-0.174653
C	1.774372	-2.143820	2.537676
C	1.434022	-1.054222	3.247625
H	2.592386	-2.125061	1.811179
H	1.283225	-3.107553	2.700782
H	0.661954	-1.091739	4.021843
H	1.972547	-0.106726	3.127963

C	-3.372440	4.118074	-0.635323
H	-2.996817	2.513798	-2.027637
C	-2.412176	3.867144	1.574649
H	-1.283479	2.064731	1.920909
C	-3.168584	4.605707	0.661220
H	-3.966909	4.692225	-1.350086
H	-2.257563	4.241250	2.589483
H	-3.605667	5.561729	0.959616
C	-1.684002	-0.703604	2.365952
C	-2.181245	-1.979541	3.054901
C	-3.037884	-2.910420	2.182644
C	-2.464464	-3.311757	0.812150
C	-0.964608	-3.676819	0.784518
C	-0.059649	-2.588336	0.211184
H	-1.324015	0.024295	3.126838
H	-2.532217	-0.209415	1.858907
H	-1.335997	-2.556283	3.464609
H	-2.790046	-1.712556	3.940196
H	-3.240108	-3.823857	2.770153
H	-4.023175	-2.439727	2.014029
H	-2.637810	-2.499262	0.093633
H	-3.060762	-4.159283	0.436607
H	-0.622988	-3.967372	1.793968
H	-0.824141	-4.587348	0.171086
H	-0.327059	-2.381847	-0.841268
H	1.003444	-2.892706	0.239909
C	1.157808	-1.709718	3.266621
C	2.180504	-1.179266	2.569942
H	0.866525	-2.755115	3.131248
H	0.641630	-1.150895	4.051891
H	2.541336	-0.162217	2.759886
H	2.757026	-1.774935	1.856868

^{4}9A-15
Geometry with 77 atoms:
Total energy: -3045.591674070

Cr	-0.077840	-0.801032	1.066795
P	1.880165	0.117322	-0.439583
P	-1.350718	0.604005	-0.579994
C	-0.216376	1.127975	-1.976111
C	1.033692	0.247907	-2.095156
H	-0.780441	1.147422	-2.920914
H	0.069823	2.166733	-1.750442
H	0.770038	-0.773374	-2.409616
H	1.731470	0.660350	-2.841070
C	3.368417	-0.910365	-0.710856
C	4.451464	-0.790420	0.181544
C	3.411042	-1.902499	-1.706055
C	5.554391	-1.639610	0.072998
H	4.441119	-0.022757	0.960031
C	4.518201	-2.750707	-1.809092
H	2.585987	-2.024432	-2.410113
C	5.590018	-2.623120	-0.921808
H	6.390554	-1.531683	0.768163
H	4.540868	-3.514486	-2.590311
H	6.453096	-3.287847	-1.004948
C	2.486764	1.822693	-0.155213
C	3.592733	2.349264	-0.846422
C	1.770660	2.648783	0.726760
C	3.969381	3.679876	-0.654313
H	4.163802	1.716824	-1.530853
C	2.143903	3.983604	0.910018
H	0.906778	2.256852	1.269196
C	3.244728	4.498855	0.220509
H	4.831406	4.082010	-1.192258
H	1.573504	4.618378	1.592299
H	3.541548	5.540566	0.364845
C	-2.734072	-0.298546	-1.364089
C	-4.000469	-0.287500	-0.753952
C	-2.521578	-1.103060	-2.496458
C	-5.034162	-1.072610	-1.268538
H	-4.183958	0.337239	0.122801
C	-3.560317	-1.886064	-3.007105
H	-1.547588	-1.128475	-2.989847
C	-4.815734	-1.876285	-2.392160
H	-6.015363	-1.055749	-0.788274
H	-3.385656	-2.507236	-3.888815
H	-5.625398	-2.492205	-2.790645
C	-2.076639	2.173628	0.019857
C	-2.742137	3.025096	-0.880846
C	-1.944264	2.558810	1.362996

^{4}9A-16
Geometry with 77 atoms:
Total energy: -3045.590022430

Cr	-0.026594	-0.753036	1.126604
P	1.888848	0.039555	-0.468730
P	-1.302354	0.563458	-0.623172
C	-0.173539	1.048614	-2.038273
C	1.079322	0.173050	-2.139436
H	-0.745350	1.042350	-2.978569
H	0.113123	2.093027	-1.840425
H	0.839553	-0.849474	-2.470891
H	1.792895	0.593522	-2.865453
C	3.399040	-0.956990	-0.736075
C	3.307419	-2.181466	-1.424736
C	4.625612	-0.587105	-0.156142
C	4.427784	-3.007342	-1.544791
H	2.360703	-2.502022	-1.865748
C	5.741178	-1.420242	-0.276172
H	4.717008	0.356057	0.386986
C	5.646158	-2.629665	-0.970945
H	4.346841	-3.952119	-2.087720
H	6.689911	-1.119434	0.175118
H	6.520434	-3.278233	-1.064323
C	2.443232	1.757322	-0.144682
C	3.298566	2.441498	-1.027833
C	1.948264	2.429809	0.984675
C	3.644352	3.771406	-0.781875
H	3.701583	1.931356	-1.906553
C	2.290976	3.763364	1.227785
H	1.283328	1.917024	1.684429
C	3.139165	4.434355	0.343676
H	4.310779	4.295161	-1.471440
H	1.892877	4.276436	2.106360
H	3.408895	5.476671	0.530459
C	-2.660961	-0.386082	-1.395854
C	-3.953462	-0.338022	-0.845997
C	-2.399375	-1.257032	-2.467308
C	-4.965447	-1.149760	-1.363567
H	-4.173334	0.332418	-0.012616
C	-3.415569	-2.066586	-2.980301
H	-1.401645	-1.318442	-2.907098
C	-4.698891	-2.016995	-2.427851
H	-5.967756	-1.104669	-0.931174
H	-3.201880	-2.739459	-3.814243
H	-5.491923	-2.652973	-2.828265
C	-2.058921	2.145952	-0.102851
C	-2.822430	2.893971	-1.017857
C	-1.858466	2.640692	1.194681

^{4}9A-17
Geometry with 77 atoms:
Total energy: -3045.593721960

Cr	-0.188668	0.686328	1.130488
P	1.712536	-0.080369	-0.647079
P	-1.605536	-0.184288	-0.722338
C	-0.602264	0.008543	-2.279661
C	0.752010	-0.691582	-2.128581
H	-1.165436	-0.398137	-3.134397
H	-0.465863	1.086699	-2.460363
H	0.606114	-1.770400	-1.968280
H	1.355868	-0.602071	-3.043598
C	2.799086	-1.518166	-0.263017
C	2.179108	-2.739282	0.066918
C	4.201317	-1.444248	-0.255907
C	2.945566	-3.860078	0.390144
H	1.089727	-2.824965	0.069543
C	4.964402	-2.568644	0.076186
H	4.710300	-0.515594	-0.518777
C	4.341889	-3.776547	0.400396
H	2.447810	-4.800773	0.638216
H	6.054867	-2.497382	0.073631
H	4.942198	-4.652488	0.658008
C	2.843265	1.236761	-1.240493
C	2.924180	1.662226	-2.575170
C	3.622451	1.893503	-0.268037
C	3.771638	2.718030	-2.929947
H	2.331967	1.180426	-3.355462
C	4.478740	2.935229	-0.627109
H	3.564211	1.583694	0.779452
C	4.551873	3.353202	-1.960900
H	3.823574	3.040563	-3.972690
H	5.086207	3.426743	0.136756
H	5.215161	4.174473	-2.242420
C	-2.049033	-1.960000	-0.695379
C	-2.735099	-2.536257	-1.779788
C	-1.694148	-2.757245	0.403913
C	-3.046156	-3.896358	-1.766624
H	-3.035913	-1.919866	-2.631032
C	-2.010658	-4.120203	0.413188
H	-1.174491	-2.311164	1.252745
C	-2.681969	-4.690033	-0.671359
H	-3.579197	-4.339705	-2.611186
H	-1.733493	-4.734472	1.273293
H	-2.929031	-5.754487	-0.663678
C	-3.178799	0.700026	-1.025218
C	-3.282239	1.761030	-1.941333
C	-4.297460	0.353234	-0.245733

C	-4.487364	2.457691	-2.077497
H	-2.433372	2.055842	-2.561054
C	-5.497511	1.051917	-0.387028
H	-4.233864	-0.469478	0.470777
C	-5.595157	2.106041	-1.301839
H	-4.558696	3.276565	-2.797575
H	-6.361264	0.770694	0.220198
H	-6.535764	2.651019	-1.411655
C	-1.859611	1.072832	2.315603
C	-1.615464	1.772254	3.660700
C	-0.816132	0.963334	4.693534
C	0.701508	0.918309	4.468626
C	1.157006	0.495257	3.064422
C	0.490672	-0.707888	2.445278
H	-2.568406	1.663172	1.710189
H	-2.346844	0.095705	2.491260
H	-1.118655	2.751048	3.510148
H	-2.594586	2.019239	4.113624
H	-0.986390	1.385963	5.697614
H	-1.221878	-0.062770	4.732473
H	1.152247	0.215250	5.189386
H	1.133732	1.909187	4.693712
H	0.997850	1.433134	2.403821
H	2.256420	0.424701	3.020007
H	-0.282619	-1.174552	3.066600
H	1.185199	-1.457241	2.051158
C	-0.815151	3.290499	0.448868
C	0.394614	3.127260	-0.109950
H	-0.929442	3.670280	1.467732
H	-1.738090	3.113104	-0.110383
H	0.512900	2.824056	-1.153794
H	1.319307	3.368092	0.422291

C	-4.303851	2.187019	-2.107543
H	-2.175789	2.024481	-2.359343
C	-5.382723	0.422976	-0.850284
H	-4.102086	-1.148693	-0.118001
C	-5.461653	1.623447	-1.563671
H	-4.360222	3.122343	-2.669476
H	-6.284956	-0.024455	-0.426660
H	-6.426364	2.118611	-1.697657
C	-0.595499	2.421168	0.910185
C	-1.589836	3.147758	1.813203
C	-2.987840	2.500176	1.900596
C	-3.228822	1.658506	3.163807
C	-2.124413	0.655875	3.528074
C	-1.720032	-0.275255	2.381494
H	0.406658	2.879599	0.988245
H	-0.916000	2.485715	-0.146301
H	-1.166871	3.263406	2.827529
H	-1.693051	4.182545	1.434518
H	-3.764357	3.281627	1.862978
H	-3.152137	1.881488	1.004629
H	-4.180091	1.110651	3.039747
H	-3.377735	2.335245	4.024177
H	-1.245612	1.208366	3.910287
H	-2.478698	0.064839	4.394045
H	-2.612888	-0.600217	1.820767
H	-1.244063	-1.199660	2.773446
C	1.375467	-0.010164	3.316867
C	1.568383	1.284662	3.011650
H	1.988239	-0.798282	2.864353
H	0.647778	-0.315103	4.073972
H	1.002868	2.081700	3.503862
H	2.344828	1.596538	2.306119

C	4.618417	-1.409987	-2.268298
H	2.490808	-1.462293	-2.561544
C	5.455307	0.221967	-0.689554
H	3.981508	1.482257	0.252216
C	5.690713	-0.817276	-1.595433
H	4.796833	-2.221047	-2.978345
H	6.289820	0.691105	-0.162990
H	6.710617	-1.164285	-1.777598
C	0.487990	-2.437237	0.219548
C	1.382287	-3.451490	0.931316
C	2.828293	-2.975349	1.190523
C	3.127706	-2.546719	2.635193
C	2.123680	-1.576147	3.275410
C	1.783132	-0.363179	2.404217
H	-0.532268	-2.835153	0.071532
H	0.900943	-2.223553	-0.783433
H	0.917773	-3.776184	1.879674
H	1.408655	-4.367095	0.309860
H	3.537811	-3.775936	0.924034
H	3.057826	-2.143282	0.506757
H	4.130282	-2.083414	2.654156
H	3.196948	-3.445336	3.274105
H	1.205298	-2.126506	3.549290
H	2.547170	-1.247020	4.243561
H	2.697066	0.036153	1.932244
H	1.365874	0.458486	3.029398
C	-1.380827	-0.800119	3.209399
C	-1.494072	-2.011091	2.636969
H	-2.055918	0.021027	2.942636
H	-0.668066	-0.616068	4.018793
H	-0.869955	-2.853700	2.947246
H	-2.249423	-2.218503	1.874073

^{4}9A-18
Geometry with 77 atoms:
Total energy: -3045.590354100

Cr	-0.197366	0.428514	1.203262
P	1.881006	0.123333	-0.519227
P	-1.363340	-0.394190	-0.830825
C	-0.266254	-0.082602	-2.301174
C	1.125127	-0.671200	-2.037509
H	-0.726210	-0.522342	-3.200062
H	-0.205909	1.006268	-2.458519
H	1.057043	-1.757883	-1.879533
H	1.792519	-0.509412	-2.897025
C	3.027320	-1.116457	0.203682
C	4.169272	-0.680304	0.902774
C	2.693307	-2.482685	0.236376
C	4.960602	-1.591503	1.606090
H	4.450460	0.375450	0.893718
C	3.489472	-3.390745	0.941258
H	1.810389	-2.856729	-0.285956
C	4.623541	-2.949023	1.628713
H	5.847300	-1.237804	2.137895
H	3.221134	-4.450097	0.948088
H	5.244992	-3.660338	2.177802
C	2.952390	1.432609	-1.230484
C	4.127913	1.107779	-1.934340
C	2.562063	2.777016	-1.126312
C	4.898951	2.115950	-2.513989
H	4.446843	0.066118	-2.022289
C	3.336301	3.784132	-1.713255
H	1.649997	3.042665	-0.590119
C	4.504853	3.455455	-2.403813
H	5.812027	1.856245	-3.055438
H	3.023904	4.827573	-1.626098
H	5.111988	4.242177	-2.858367
C	-1.613350	-2.208365	-0.882797
C	-2.293796	-2.805126	-1.959773
C	-1.077090	-3.022367	0.127739
C	-2.429142	-4.192885	-2.021048
H	-2.728838	-2.183545	-2.746552
C	-1.210666	-4.413008	0.061440
H	-0.559026	-2.575394	0.978364
C	-1.886187	-4.998275	-1.012420
H	-2.962561	-4.649107	-2.858443
H	-0.791968	-5.036940	0.854620
H	-1.996190	-6.084228	-1.063085
C	-2.981592	0.354817	-1.215243
C	-3.067289	1.560139	-1.933408
C	-4.150853	-0.210334	-0.674844

^{4}9A-19
Geometry with 77 atoms:
Total energy: -3045.591375020

Cr	0.196773	-0.601361	1.114982
P	-1.838736	0.014942	-0.498024
P	1.371258	0.584708	-0.696152
C	0.365722	0.391134	-2.247038
C	-1.085109	0.823923	-2.007462
H	0.824588	0.973233	-3.061051
H	0.423707	-0.668766	-2.536635
H	-1.131395	1.906000	-1.807861
H	-1.714237	0.634542	-2.890998
C	-3.084871	1.239180	0.061300
C	-2.687645	2.174263	1.034088
C	-4.383339	1.313250	-0.471706
C	-3.572734	3.163514	1.470466
H	-1.675065	2.144161	1.446192
C	-5.268065	2.299236	-0.027272
H	-4.708412	0.598226	-1.230685
C	-4.866378	3.223163	0.943591
H	-3.251757	3.885782	2.224852
H	-6.277141	2.347600	-0.443869
H	-5.562938	3.990799	1.289282
C	-2.777531	-1.434312	-1.108127
C	-2.400265	-2.109187	-2.281708
C	-3.819299	-1.965512	-0.323405
C	-3.053849	-3.284547	-2.664135
H	-1.593400	-1.729035	-2.911045
C	-4.471088	-3.138191	-0.711046
H	-4.141190	-1.452310	0.586547
C	-4.088628	-3.802700	-1.881161
H	-2.751465	-3.795781	-3.581342
H	-5.284614	-3.532269	-0.097124
H	-4.598980	-4.720392	-2.182890
C	1.451192	2.397114	-0.432626
C	1.806370	3.268389	-1.477896
C	1.141257	2.929522	0.829284
C	1.835249	4.647125	-1.262493
H	2.070164	2.872845	-2.461970
C	1.173048	4.311174	1.043132
H	0.892825	2.265303	1.660225
C	1.515555	5.170364	-0.003521
H	2.112072	5.317727	-2.079500
H	0.934018	4.714109	2.030232
H	1.540037	6.250211	0.161615
C	3.069896	0.073025	-1.126839
C	3.312072	-0.972813	-2.034454
C	4.153015	0.667228	-0.454687

^{4}9A-20
Geometry with 77 atoms:
Total energy: -3045.593841670

Cr	-0.150030	-0.267533	1.302355
P	1.744946	0.202273	-0.517338
P	-1.683269	0.205171	-0.617736
C	-0.610668	0.865932	-1.984522
C	0.742509	0.146976	-2.088001
H	-1.147777	0.814029	-2.943758
H	-0.470758	1.934590	-1.758806
H	0.604533	-0.925607	-2.295422
H	1.339552	0.546378	-2.922656
C	3.150543	-0.924804	-0.910543
C	2.907702	-2.309322	-0.984513
C	4.451972	-0.448957	-1.145547
C	3.943623	-3.195351	-1.287488
H	1.908202	-2.706600	-0.807577
C	5.486628	-1.341676	-1.441662
H	4.668444	0.619391	-1.101584
C	5.237304	-2.714639	-1.512815
H	3.737438	-4.267143	-1.341358
H	6.493645	-0.956875	-1.620962
H	6.048758	-3.409029	-1.743824
C	2.504223	1.871914	-0.462555
C	3.267223	2.199027	0.674536
C	2.349872	2.832270	-1.475321
C	3.863955	3.455121	0.793805
H	3.408537	1.459239	1.468225
C	2.937477	4.095568	-1.346883
H	1.776513	2.609816	-2.376993
C	3.693727	4.409835	-0.215024
H	4.459723	3.691780	1.678705
H	2.807000	4.834476	-2.141346
H	4.152805	5.396602	-0.118774
C	-2.537974	-1.272504	-1.293144
C	-2.257051	-1.820245	-2.553778
C	-3.497602	-1.892262	-0.472493
C	-2.926926	-2.970936	-2.984891
H	-1.521336	-1.363779	-3.218164
C	-4.168126	-3.034611	-0.909656
H	-3.725838	-1.478325	0.513296
C	-3.881319	-3.579060	-2.166766
H	-2.700919	-3.389366	-3.968744
H	-4.915537	-3.503894	-0.265423
H	-4.403572	-4.476413	-2.507210
C	-3.027936	1.431520	-0.408250
C	-3.470603	2.244499	-1.465008
C	-3.654406	1.526004	0.846440

C	-4.519973	3.144716	-1.262645
H	-3.009017	2.179389	-2.452706
C	-4.710173	2.420511	1.040428
H	-3.307414	0.904875	1.675730
C	-5.141097	3.233537	-0.012561
H	-4.857302	3.776275	-2.088170
H	-5.192719	2.487126	2.018477
H	-5.962621	3.937655	0.140299
C	-1.192160	-0.529282	3.036726
C	0.189258	-0.773061	3.588451
C	0.534992	-2.175730	4.105380
C	0.185320	-3.340825	3.169936
C	0.671065	-3.185829	1.720437
C	-0.206212	-2.277456	0.855533
H	-1.685292	0.373736	3.421592
H	-1.868660	-1.392023	3.066609
H	0.998932	-0.559842	2.776677
H	0.485954	-0.014054	4.329934
H	1.616061	-2.203373	4.328281
H	0.017096	-2.314551	5.069501
H	-0.906528	-3.503679	3.160858
H	0.618468	-4.255921	3.606124
H	1.725655	-2.849743	1.713568
H	0.689576	-4.192143	1.259832
H	-1.262130	-2.579974	0.940315
H	0.051623	-2.371518	-0.213063
C	0.321389	2.372750	2.549633
C	-0.308814	2.725466	1.420971
H	1.410532	2.293603	2.599176
H	-0.228222	2.211807	3.480940
H	-1.391762	2.867036	1.392117
H	0.247479	2.950608	0.506613

C	-4.272939	2.618989	1.403691
H	-4.228838	0.650003	0.527954
C	-2.330723	4.008424	1.018587
H	-0.748053	3.147386	-0.149389
C	-3.595532	3.828961	1.586684
H	-5.262142	2.471823	1.843918
H	-1.794282	4.949987	1.158260
H	-4.052946	4.630735	2.171132
C	-1.939520	-1.497160	1.940515
C	-1.744343	-2.451638	3.127251
C	-1.106269	-3.804451	2.777325
C	0.416501	-3.788402	2.591158
C	0.970132	-2.738144	1.617924
C	0.291592	-2.593673	0.278138
H	-2.550437	-0.630661	2.246743
H	-2.515149	-2.014461	1.152752
H	-1.153504	-1.972478	3.932355
H	-2.732191	-2.653842	3.583323
H	-1.331174	-4.531190	3.575491
H	-1.593630	-4.202782	1.870178
H	0.745646	-4.777976	2.231017
H	0.900502	-3.642672	3.573024
H	0.943365	-1.734982	2.197251
H	2.059152	-2.856511	1.510695
H	-0.554456	-3.274007	0.128709
H	0.973504	-2.630310	-0.581895
C	-0.565098	0.958948	3.062111
C	0.607385	1.287542	2.494426
H	-1.494686	1.453019	2.766051
H	-0.628319	0.239816	3.883135
H	1.553912	0.859952	2.839135
H	0.675626	2.070969	1.735875

C	-5.375543	0.645424	-1.092714
H	-4.226006	-1.082107	-0.515967
C	-4.117712	2.576490	-1.827555
H	-1.978587	2.391327	-1.815889
C	-5.345258	1.960925	-1.564376
H	-6.331236	0.156491	-0.889387
H	-4.086592	3.603384	-2.199238
H	-6.277810	2.505862	-1.729330
C	-0.622626	2.243541	1.393376
C	-1.656550	2.746344	2.396691
C	-3.102872	2.240829	2.213594
C	-3.505674	0.998686	3.022405
C	-2.907905	-0.353323	2.613735
C	-1.388956	-0.458014	2.729531
H	0.362151	2.705644	1.600171
H	-0.908377	2.523416	0.363193
H	-1.322121	2.529032	3.427624
H	-1.668322	3.851888	2.328939
H	-3.784806	3.052939	2.516415
H	-3.304068	2.071899	1.142671
H	-4.604867	0.906800	2.973182
H	-3.269388	1.182025	4.087892
H	-3.378323	-1.124081	3.254849
H	-3.237446	-0.598041	1.590232
H	-1.071922	-1.524870	2.738553
H	-1.049651	-0.030004	3.692138
C	1.806497	-0.392850	3.292451
C	1.786244	0.948784	3.223976
H	2.503345	-0.984934	2.690100
H	1.164911	-0.938074	3.990901
H	1.132672	1.547865	3.865780
H	2.472683	1.495858	2.569242

^{4}9A-21
Geometry with 77 atoms:
Total energy: -3045.593657370

Cr	-0.212929	-0.764660	1.018004
P	1.736268	0.200250	-0.566494
P	-1.584707	0.337344	-0.706034
C	-0.498512	1.025211	-2.062391
C	0.820315	0.250190	-2.180723
H	-1.061385	0.982095	-3.006747
H	-0.317576	2.087727	-1.849434
H	0.626306	-0.801018	-2.447552
H	1.449401	0.674430	-2.978215
C	3.170621	-0.913865	-0.851789
C	3.560632	-1.352934	-2.127874
C	3.910912	-1.332242	0.268638
C	4.669548	-2.192113	-2.274813
H	3.012720	-1.046200	-3.020478
C	5.024672	-2.160737	0.117273
H	3.616648	-1.011707	1.271351
C	5.404765	-2.594789	-1.156527
H	4.962140	-2.528127	-3.272656
H	5.592388	-2.473373	0.997095
H	6.272332	-3.247944	-1.276791
C	2.517177	1.868072	-0.415861
C	2.350311	2.884952	-1.371594
C	3.301795	2.136231	0.721684
C	2.941948	4.139414	-1.185706
H	1.773044	2.714281	-2.281235
C	3.899404	3.384607	0.899980
H	3.458479	1.361832	1.476139
C	3.715117	4.393946	-0.051011
H	2.802292	4.917344	-1.940485
H	4.509575	3.571076	1.787038
H	4.177494	5.373683	0.090856
C	-2.867344	-0.605555	-1.607765
C	-3.897756	0.058830	-2.298223
C	-2.770123	-2.003596	-1.687065
C	-4.819545	-0.671985	-3.049750
H	-3.986289	1.146511	-2.243958
C	-3.693286	-2.729579	-2.446018
H	-1.972811	-2.523751	-1.156413
C	-4.718429	-2.066292	-3.125110
H	-5.620708	-0.150944	-3.579593
H	-3.610960	-3.817647	-2.501975
H	-5.442333	-2.634906	-3.714011
C	-2.421699	1.767658	0.076520
C	-3.690765	1.591327	0.657834
C	-1.743576	2.984310	0.270346

^{4}9A-22
Geometry with 77 atoms:
Total energy: -3045.590194310

Cr	-0.085827	0.273260	1.342580
P	1.914200	0.149747	-0.471564
P	-1.375697	-0.292854	-0.748683
C	-0.270546	0.105831	-2.198551
C	1.109059	-0.530951	-2.014133
H	-0.758757	-0.247265	-3.120206
H	-0.189612	1.201888	-2.273280
H	1.019740	-1.623759	-1.914454
H	1.755804	-0.334598	-2.882550
C	3.153141	-1.108322	0.026746
C	2.752193	-2.453643	0.141674
C	4.436817	-0.740942	0.466360
C	3.624519	-3.410911	0.664445
H	1.753220	-2.767754	-0.172577
C	5.304803	-1.702998	0.992272
H	4.766016	0.298144	0.398606
C	4.903613	-3.038396	1.091533
H	3.302304	-4.452505	0.738572
H	6.302081	-1.404437	1.324713
H	5.585328	-3.787462	1.501283
C	2.856372	1.591921	-1.095254
C	2.507179	2.884078	-0.671999
C	3.897615	1.429150	-2.029081
C	3.188414	3.998675	-1.173751
H	1.698216	3.024972	0.046449
C	4.577338	2.542808	-2.523198
H	4.185558	0.428565	-2.362180
C	4.222920	3.829127	-2.096570
H	2.909009	5.000616	-0.839142
H	5.387514	2.408360	-3.244144
H	4.757321	4.699306	-2.485671
C	-1.683331	-2.086673	-0.974899
C	-1.213380	-3.004308	-0.021391
C	-2.327565	-2.566663	-2.130493
C	-1.377819	-4.379222	-0.219638
H	-0.725290	-2.651910	0.889115
C	-2.494843	-3.938661	-2.323032
H	-2.710082	-1.866859	-2.877489
C	-2.018296	-4.846767	-1.369615
H	-1.010309	-5.083284	0.530647
H	-3.001117	-4.301902	-3.220620
H	-2.151827	-5.920295	-1.523777
C	-2.946873	0.560735	-1.135731
C	-4.184990	-0.053622	-0.879214
C	-2.924162	1.883954	-1.613194

^{4}9A-23
Geometry with 77 atoms:
Total energy: -3045.591355340

Cr	-0.082496	-0.372509	1.225835
P	1.635129	0.144636	-0.681366
P	-1.721280	0.149962	-0.597224
C	-0.765794	0.558072	-2.152230
C	0.627399	-0.080987	-2.243362
H	-1.378133	0.302701	-3.031412
H	-0.688458	1.654724	-2.152753
H	0.551109	-1.166596	-2.405007
H	1.174720	0.341420	-3.100045
C	3.077520	-0.965394	-0.861918
C	3.761885	-1.327882	0.312182
C	3.524705	-1.461204	-2.097346
C	4.874114	-2.170033	0.252898
H	3.422717	-0.948813	1.280999
C	4.630491	-2.315262	-2.151904
H	3.021829	-1.185103	-3.026283
C	5.306180	-2.669950	-0.980374
H	5.400698	-2.441677	1.171005
H	4.967921	-2.701753	-3.116667
H	6.170547	-3.336705	-1.027753
C	2.326796	1.843101	-0.849070
C	3.706519	2.067882	-0.992748
C	1.457647	2.951161	-0.818987
C	4.201104	3.370161	-1.113943
H	4.403527	1.228168	-1.013958
C	1.955601	4.249039	-0.950316
H	0.383147	2.812424	-0.688412
C	3.329789	4.462364	-1.096799
H	5.276568	3.528626	-1.225805
H	1.265736	5.096349	-0.931266
H	3.720179	5.478254	-1.193947
C	-2.651848	-1.388758	-0.941390
C	-2.408321	-2.193562	-2.064960
C	-3.583678	-1.815533	0.023919
C	-3.086348	-3.407841	-2.219858
H	-1.688444	-1.890190	-2.827162
C	-4.266928	-3.020433	-0.141895
H	-3.770278	-1.202960	0.909763
C	-4.015154	-3.822357	-1.262142
H	-2.886559	-4.029717	-3.095702
H	-4.993060	-3.339751	0.609429
H	-4.543533	-4.770539	-1.386653
C	-2.963947	1.492734	-0.518582
C	-2.612037	2.704422	0.102797
C	-4.225658	1.365268	-1.123808

C	-3.510831	3.774120	0.112671
H	-1.641583	2.816373	0.588776
C	-5.121595	2.437321	-1.104261
H	-4.513795	0.430641	-1.609418
C	-4.766524	3.641586	-0.488341
H	-3.231044	4.711106	0.600267
H	-6.102036	2.329866	-1.574694
H	-5.470975	4.476875	-0.474216
C	0.083116	1.437304	2.174643
C	0.981316	1.473379	3.413046
C	0.439405	0.708408	4.629824
C	0.643979	-0.811928	4.588616
C	0.213537	-1.505886	3.290344
C	-1.157725	-1.209720	2.737409
H	0.465558	2.131093	1.410629
H	-0.945777	1.738035	2.435030
H	2.001600	1.117850	3.167612
H	1.115382	2.531736	3.707699
H	0.924538	1.084340	5.545532
H	-0.633244	0.943150	4.743601
H	0.088011	-1.277845	5.419695
H	1.710489	-1.037937	4.764910
H	1.040250	-1.209633	2.523552
H	0.415952	-2.586955	3.352822
H	-1.760892	-0.507027	3.325467
H	-1.742897	-2.094969	2.457027
C	0.597706	-3.221282	-0.230793
C	-0.384037	-3.608617	0.590202
H	1.649438	-3.245334	0.066437
H	0.385550	-2.915837	-1.258848
H	-1.430064	-3.617886	0.274313
H	-0.172839	-3.963423	1.603079

^{4}9B-01

Geometry with 85 atoms:

Total energy: -3274.499967820

Cr	-0.674975	-0.532424	1.214905
C	-1.068237	-2.480982	0.684076
C	-2.472717	-3.056567	0.491692
C	-3.317715	-3.285222	1.752528
C	-4.047878	-2.074032	2.348414
C	-3.205439	-1.052227	3.121486
C	-2.390000	-0.067449	2.282559
H	-2.000872	0.736453	2.937714
H	-3.069168	0.437302	1.571299
H	-2.561379	-1.595037	3.836961
H	-3.900682	-0.467948	3.756269
H	-4.815699	-2.462931	3.039965
H	-4.604741	-1.555763	1.545135
H	-4.087715	-4.034487	1.499071
H	-2.693631	-3.759658	2.534327
H	-3.053163	-2.436230	-0.211573
H	-2.367243	-4.036904	-0.013512
H	-0.496080	-2.606454	-0.254213
H	-0.527982	-3.068154	1.454126
P	-1.546525	0.306159	-0.900995
C	-3.213937	-0.064152	-1.540911
C	-3.409722	-1.060288	-2.513160
C	-4.702337	-1.391540	-2.928275
C	-5.807823	-0.737466	-2.377609
C	-5.618831	0.257285	-1.412387
C	-4.330295	0.593898	-0.993777
H	-4.195500	1.376716	-0.244048
H	-6.479092	0.775561	-0.982141
H	-6.817491	-1.000188	-2.702353
H	-4.843523	-2.167091	-3.684899
H	-2.562487	-1.593436	-2.948123
C	-1.455330	2.130458	-0.773874
C	-1.961760	2.962242	-1.784985
C	-1.861692	4.350257	-1.692011
C	-1.248944	4.915998	-0.571012
C	-0.737477	4.110963	0.449984
C	-0.836060	2.715899	0.350837
O	-0.327975	1.870257	1.310408
C	0.145676	2.439094	2.537284
H	0.412387	1.602952	3.190668
H	1.041212	3.054204	2.364956
H	-0.644106	3.033444	3.021634
H	-0.262649	4.579631	1.310287
H	-1.165205	6.001722	-0.481269
H	-2.262292	4.984936	-2.484944
H	-2.452709	2.510640	-2.650697
C	-0.361820	-0.102280	-2.271360
C	1.047441	0.384974	-1.926967
P	1.621543	-0.262760	-0.265957
C	2.668861	-1.712999	-0.671742
C	2.376648	-2.971087	-0.124787
C	3.174201	-4.086526	-0.395513
C	4.286758	-3.943267	-1.225261
C	4.606195	-2.702938	-1.786156
C	3.802732	-1.584546	-1.518309
O	4.037234	-0.353617	-2.022164
C	5.213276	-0.096854	-2.773350
H	5.227551	-0.668870	-3.717220
H	5.199851	0.976564	-3.004242
H	6.121625	-0.327613	-2.190914
H	5.479179	-2.616304	-2.432719
H	4.921063	-4.805490	-1.446186
H	2.925564	-5.056350	0.040014
H	1.504775	-3.083976	0.518323
C	2.818026	0.989251	0.360926
C	2.633051	2.365953	0.152736
C	3.506433	3.295388	0.726328
C	4.572149	2.866328	1.522610
C	4.763055	1.497355	1.736835
C	3.895013	0.566461	1.161165
H	4.069307	-0.499781	1.324897
H	5.597885	1.149301	2.350421
H	5.254504	3.593794	1.968809
H	3.351068	4.362042	0.544270
H	1.808235	2.736127	-0.458019
H	1.771659	0.081307	-2.694009
H	1.068148	1.483501	-1.887732
H	-0.717757	0.353129	-3.209116
H	-0.379293	-1.196091	-2.404294
C	1.314134	-1.081380	2.969526
C	0.154357	-1.239543	3.632211
H	-0.355660	-2.205105	3.666306
H	-0.285274	-0.435895	4.229388
H	1.791694	-1.916062	2.449353
H	1.875759	-0.142188	2.990142

^{4}9B-02

Geometry with 85 atoms:

Total energy: -3274.498551170

Cr	-0.417852	-0.498341	1.227457
C	-0.372118	-2.493489	0.738587
C	-1.547894	-3.193644	0.056577
C	-2.687198	-3.653696	0.973080
C	-3.515611	-2.581821	1.694664
C	-2.815322	-1.793413	2.819163
C	-2.128525	-0.491928	2.400573
H	-1.806717	0.069650	3.298980
H	-2.869095	0.160717	1.903925
H	-2.102540	-2.461676	3.336489
H	-3.579255	-1.547257	3.582241
H	-4.386145	-3.098018	2.134405
H	-3.934599	-1.876965	0.956218
H	-3.381687	-4.260954	0.365726
H	-2.269491	-4.346154	1.728722
H	-1.967620	-2.562158	-0.745581
H	-1.169103	-4.093961	-0.465735
H	0.530334	-2.583804	0.108677
H	-0.136414	-3.005605	1.690360
P	-1.672288	0.320778	-0.719147
C	-3.419639	-0.052872	-1.099334
C	-3.766525	-1.030880	-2.047462
C	-5.107880	-1.363057	-2.256612
C	-6.113561	-0.723733	-1.526515
C	-5.775604	0.259229	-0.590470
C	-4.437814	0.594226	-0.376008
H	-4.189434	1.367598	0.353911
H	-6.557931	0.768141	-0.022360
H	-7.161216	-0.987634	-1.689743
H	-5.365474	-2.126107	-2.994883
H	-2.998763	-1.545105	-2.628001
C	-1.611182	2.145888	-0.555802
C	-2.150441	2.973803	-1.554274
C	-2.077818	4.362339	-1.456184
C	-1.458188	4.935526	-0.342392
C	-0.918210	4.134895	0.665914
C	-0.990108	2.738946	0.560958
O	-0.460773	1.904244	1.524521
C	-0.193396	2.463910	2.816125
H	0.110915	1.636172	3.462925
H	0.625241	3.198638	2.773505
H	-1.098635	2.935261	3.228848
H	-0.439573	4.607360	1.521916
H	-1.392410	6.022104	-0.249253
H	-2.504447	4.992292	-2.239264
H	-2.645662	2.517516	-2.415340
C	-0.733730	0.009593	-2.289327
C	0.680874	0.585655	-2.176367
P	1.585616	0.025903	-0.636908
C	2.508538	-1.464007	-1.194563
C	2.155914	-2.203516	-2.331922
C	2.843644	-3.370005	-2.681621
C	3.903433	-3.806936	-1.886828
C	4.276973	-3.092171	-0.744295
C	3.577186	-1.931380	-0.390481
O	3.852775	-1.186274	0.707821
C	4.963337	-1.501291	1.530112
H	5.003056	-0.724387	2.305385
H	4.847570	-2.487353	2.012866
H	5.907003	-1.482640	0.958621
H	5.106883	-3.447778	-0.133754
H	4.451095	-4.714768	-2.151383
H	2.551371	-3.929041	-3.572918
H	1.331778	-1.875650	-2.966954
C	2.878523	1.323293	-0.480216
C	3.885256	1.475703	-1.447479
C	4.840458	2.485706	-1.312439
C	4.800799	3.350265	-0.212185
C	3.803603	3.200385	0.755635
C	2.847251	2.189054	0.621832
H	2.073218	2.064863	1.379460
H	3.772627	3.869899	1.619216
H	5.550609	4.138680	-0.109156
H	5.622158	2.597511	-2.068153
H	3.931860	0.796104	-2.302518
H	1.276136	0.358453	-3.073849
H	0.632872	1.682726	-2.098023
H	-1.276503	0.455350	-3.137645
H	-0.720649	-1.081140	-2.439533
C	0.611730	-1.090620	3.658452
C	1.620347	-0.886794	2.793282
H	2.157225	0.065091	2.739412
H	2.007357	-1.690500	2.164747
H	0.274105	-0.316388	4.352958
H	0.119841	-2.061851	3.754570

^{4}9B-03

Geometry with 85 atoms:

Total energy: -3274.499121670

Cr	-0.353251	-0.542033	1.183788
C	-0.312345	-2.528094	0.632041
C	-1.488114	-3.181957	-0.097135
C	-2.627278	-3.696937	0.790449
C	-3.391605	-2.679517	1.648442
C	-2.616366	-2.044504	2.820410
C	-1.912616	-0.720747	2.519528
H	-1.420495	-0.352443	3.443679
H	-2.659046	0.046935	2.239932
H	-1.892673	-2.780742	3.216063
H	-3.331405	-1.875687	3.649145
H	-4.268620	-3.206573	2.061430
H	-3.802323	-1.882503	1.007103
H	-3.357736	-4.208607	0.138672
H	-2.220995	-4.481137	1.457149
H	-1.907971	-2.503593	-0.860035
H	-1.110639	-4.047666	-0.675477
H	0.608239	-2.624588	0.032206
H	-0.126676	-3.062732	1.580764
P	-1.692662	0.303597	-0.693931
C	-3.451216	-0.062504	-1.012024
C	-3.854814	-0.972008	-2.003377
C	-5.207966	-1.289962	-2.153039
C	-6.164942	-0.704620	-1.319862
C	-5.768602	0.208933	-0.336653
C	-4.419539	0.528191	-0.180059
H	-4.119850	1.239809	0.592839
H	-6.513938	0.672566	0.313941
H	-7.221362	-0.957346	-1.438092

H -5.513170 -1.998725 -2.926453
H -3.123900 -1.441550 -2.664073
C -1.620348 2.131837 -0.559936
C -2.077858 2.947758 -1.607818
C -1.956010 4.334742 -1.543908
C -1.364496 4.918461 -0.419229
C -0.913945 4.129156 0.640228
C -1.049807 2.735198 0.575179
O -0.625912 1.911735 1.597659
C -0.608587 2.465634 2.921707
H -0.640928 1.624841 3.621736
H 0.305943 3.055406 3.092527
H -1.496714 3.093521 3.089298
H -0.451123 4.603644 1.505211
H -1.250764 6.003484 -0.360371
H -2.317660 4.956769 -2.365169
H -2.542428 2.483540 -2.481551
C -0.782613 -0.012320 -2.284590
C 0.625317 0.591160 -2.210501
P 1.558681 0.053134 -0.683385
C 2.493583 -1.427362 -1.230294
C 2.217933 -2.120503 -2.416740
C 2.908425 -3.290859 -2.747632
C 3.891701 -3.775848 -1.885109
C 4.186471 -3.106644 -0.692777
C 3.481068 -1.944320 -0.357082
O 3.674869 -1.244226 0.789545
C 4.756834 -1.570545 1.648411
H 4.639581 -2.574501 2.091002
H 5.720991 -1.516125 1.115191
H 4.749490 -0.824013 2.453215
H 4.956275 -3.501376 -0.029869
H 4.441200 -4.686657 -2.135211
H 2.679003 -3.815588 -3.677335
H 1.455824 -1.751538 -3.104799
C 2.822197 1.374156 -0.503106
C 3.997677 1.401011 -1.270699
C 4.914226 2.443203 -1.111638
C 4.665824 3.466497 -0.189468
C 3.497434 3.444576 0.577532
C 2.580920 2.399970 0.424388
H 1.673605 2.374341 1.029757
H 3.300350 4.240593 1.300223
H 5.385762 4.279752 -0.068293
H 5.828210 2.457197 -1.710796
H 4.202085 0.601704 -1.987468
H 1.205043 0.367001 -3.118647
H 0.563863 1.687676 -2.141145
H -1.351058 0.414464 -3.125846
H -0.747930 -1.104244 -2.425770
C 1.690041 -0.154824 3.057782
C 1.432628 -1.472134 3.061548
H 1.947896 -2.146355 2.374126
H 0.739037 -1.921840 3.778450
H 2.418943 0.279962 2.368871
H 1.224856 0.515043 3.785256

^{4}9B-04
Geometry with 85 atoms:
Total energy: -3274.498883230
Cr -0.383082 -0.495563 1.066942
C -0.377797 -2.369588 0.196501
C -1.546664 -3.329475 0.414137
C -1.715558 -3.904912 1.833226
C -2.639487 -3.136637 2.788291
C -2.155993 -1.782863 3.320301
C -2.043570 -0.660734 2.282952
H -2.011528 0.319502 2.797689
H -2.958593 -0.651521 1.665323
H -1.203471 -1.927139 3.864309
H -2.874944 -1.469729 4.102879
H -2.843255 -3.787568 3.656931
H -3.615679 -2.990300 2.288652
H -2.129764 -4.923061 1.738570
H -0.721309 -4.039086 2.299799
H -2.493572 -2.855950 0.102235
H -1.409697 -4.181268 -0.280660
H -0.247073 -2.193579 -0.887049
H 0.569068 -2.837683 0.524908
P -1.684229 0.368575 -0.809731
C -3.316616 -0.340625 -1.213119
C -3.430917 -1.435539 -2.087172
C -4.675069 -2.032878 -2.305366
C -5.812078 -1.550947 -1.650480
C -5.703582 -0.464833 -0.776014
C -4.463749 0.138588 -0.555531
H -4.391487 0.988066 0.127425
H -6.588946 -0.083960 -0.261266
H -6.783140 -2.021934 -1.821271
H -4.753200 -2.881421 -2.989240
H -2.554547 -1.839031 -2.597857
C -1.957148 2.164901 -0.595056
C -2.655463 2.900050 -1.567620
C -2.833409 4.276707 -1.441146
C -2.303371 4.931958 -0.326521
C -1.608138 4.223891 0.655562
C -1.432113 2.837758 0.527262
O -0.750461 2.095872 1.464574
C -0.569056 2.677740 2.759973
H 0.172967 3.491910 2.734235
H -1.524316 3.056966 3.154828
H -0.203518 1.885457 3.417995
H -1.203006 4.761677 1.511270
H -2.431112 6.011111 -0.212370
H -3.382200 4.832973 -2.203700
H -3.077572 2.377384 -2.429757
C -0.681150 0.288547 -2.371029
C 0.705221 0.902370 -2.147904
P 1.607826 0.194794 -0.670477
C 2.543611 -1.233489 -1.342729
C 2.267064 -1.821052 -2.585054
C 2.970968 -2.945481 -3.027622
C 3.973478 -3.490406 -2.225069
C 4.273890 -2.925118 -0.981671
C 3.553778 -1.810288 -0.535241
O 3.761752 -1.205567 0.662772
C 4.885978 -1.555675 1.455709
H 5.826915 -1.423575 0.894953
H 4.880973 -0.871449 2.314643
H 4.820101 -2.594668 1.822398
H 5.062498 -3.358668 -0.366741
H 4.534382 -4.364781 -2.563869
H 2.738900 -3.386128 -3.999370
H 1.497552 -1.400414 -3.233825
C 2.864043 1.498800 -0.353332
C 4.125436 1.516124 -0.969152
C 5.021825 2.553794 -0.701135
C 4.668670 3.584030 0.177714
C 3.412414 3.574375 0.790664
C 2.516290 2.533716 0.529838
H 1.535936 2.522795 1.007931
H 3.130684 4.376854 1.477242
H 5.373480 4.393239 0.384168
H 6.002617 2.559079 -1.183369
H 4.412967 0.716751 -1.656077
H 1.331257 0.817312 -3.049783
H 0.613667 1.979081 -1.933520
H -1.222379 0.812115 -3.174798
H -0.607672 -0.770729 -2.658769
C 1.116551 -0.343591 3.154146
C 1.348550 -1.605134 2.753625
H 2.145954 -1.827815 2.042571
H 0.774236 -2.446365 3.149674
H 1.737599 0.485430 2.796628
H 0.358881 -0.123866 3.912144

^{4}9B-05
Geometry with 85 atoms:
Total energy: -3274.500156640
Cr -0.368480 -0.464724 1.329178
C -0.599085 -2.478507 1.000392
C -1.817060 -3.061354 0.284849
C -3.058528 -3.300946 1.151727
C -3.721895 -2.084147 1.810179
C -2.934855 -1.396331 2.944506
C -2.044110 -0.227421 2.521398
H -1.625778 0.258624 3.425334
H -2.666920 0.545663 2.033960
H -2.345117 -2.156946 3.489978
H -3.667468 -1.021708 3.685715
H -4.686293 -2.429496 2.220060
H -3.978239 -1.338075 1.039086
H -3.816468 -3.802447 0.523735
H -2.796994 -4.029264 1.942724
H -2.099936 -2.438897 -0.581594
H -1.539590 -4.038520 -0.157083
H 0.319392 -2.734299 0.449166
H -0.508460 -2.928454 2.006066
P -1.455037 0.374298 -0.699881
C -3.239928 0.276191 -1.064383
C -3.758873 -0.699258 -1.932154
C -5.139409 -0.806412 -2.122347
C -6.010892 0.056434 -1.452075
C -5.498799 1.035960 -0.594190
C -4.121447 1.146717 -0.398828
H -3.731779 1.916702 0.270978
H -6.175778 1.717524 -0.073650
H -7.089740 -0.030940 -1.601411
H -5.533808 -1.567979 -2.799306
H -3.095125 -1.383823 -2.463296
C -1.068161 2.164342 -0.725500
C -1.327620 2.941848 -1.865540
C -0.992584 4.294233 -1.902882
C -0.392707 4.879595 -0.783694
C -0.132605 4.129403 0.364481
C -0.467328 2.768407 0.395246
O -0.225783 1.972805 1.493786
C -0.020230 2.620796 2.754146
H 0.004374 1.834743 3.515328
H 0.933905 3.168254 2.771226
H -0.851392 3.308242 2.975259
H 0.342496 4.609019 1.218686
H -0.120820 5.937700 -0.798513
H -1.200201 4.888417 -2.795076
H -1.807141 2.475945 -2.730530
C -0.574754 -0.277896 -2.194915
C 0.907922 0.105686 -2.156593
P 1.675388 -0.143680 -0.457414
C 2.894949 -1.510012 -0.629839
C 4.181599 -1.403348 -0.080171
C 5.067819 -2.484080 -0.097027
C 4.668273 -3.691648 -0.670702
C 3.394264 -3.824634 -1.231393
C 2.507045 -2.739811 -1.213904
O 1.254505 -2.782768 -1.738269
C 0.738559 -4.004698 -2.241271
H -0.293368 -3.800985 -2.555285
H 1.314262 -4.357988 -3.113865
H 0.728253 -4.789317 -1.466025
H 3.100701 -4.773022 -1.680893
H 5.351405 -4.544366 -0.690053
H 6.065412 -2.377828 0.334246
H 4.500307 -0.459756 0.367064
C 2.744397 1.337968 -0.240607
C 2.899746 1.887845 1.041817
C 3.706816 3.011421 1.243405
C 4.363612 3.603230 0.161125
C 4.222540 3.058305 -1.119737
C 3.423953 1.930112 -1.319905
H 3.340663 1.509705 -2.324861
H 4.742371 3.510953 -1.967679
H 4.990205 4.485068 0.315266
H 3.821650 3.425818 2.248327
H 2.384552 1.438163 1.890850
H 1.473390 -0.466057 -2.904446
H 1.017790 1.174372 -2.389478
H -1.056172 0.103062 -3.108967
H -0.695854 -1.369484 -2.175213
C 1.818642 -1.333701 2.757174
C 0.851160 -1.014191 3.635008
H 0.055492 -1.715565 3.899326
H 0.874511 -0.071712 4.190639
H 1.848693 -2.304350 2.255984
H 2.658516 -0.663492 2.556472

^{4}9B-06
Geometry with 85 atoms:
Total energy: -3274.498189870
Cr -0.329435 -0.542682 0.990594
C -0.390115 -2.391267 0.072784
C -1.585542 -3.319127 0.284630
C -1.765100 -3.916573 1.692786
C -2.660603 -3.139012 2.667399

C	-2.123177	-1.822119	3.238322
C	-1.969308	-0.671274	2.239325
H	-1.852589	0.283847	2.788812
H	-2.901941	-0.576144	1.656171
H	-1.173702	-2.020554	3.770268
H	-2.824486	-1.505790	4.035626
H	-2.891402	-3.804937	3.517700
H	-3.629814	-2.941671	2.171639
H	-2.211622	-4.918975	1.579289
H	-0.774547	-4.091604	2.153285
H	-2.517166	-2.810664	-0.014616
H	-1.478767	-4.160200	-0.427791
H	-0.289756	-2.189509	-1.008837
H	0.546830	-2.896698	0.373166
P	-1.643051	0.457287	-0.830290
C	-2.967094	-0.581677	-1.536641
C	-2.720225	-1.384763	-2.662402
C	-3.689341	-2.286142	-3.111580
C	-4.911371	-2.396688	-2.442813
C	-5.165303	-1.597229	-1.323467
C	-4.199865	-0.697300	-0.868733
H	-4.409474	-0.081286	0.007786
H	-6.119818	-1.676047	-0.797681
H	-5.666434	-3.103666	-2.794698
H	-3.484920	-2.905329	-3.988300
H	-1.771951	-1.324295	-3.199189
C	-2.443353	1.997744	-0.263961
C	-3.562809	2.548443	-0.905197
C	-4.163688	3.713214	-0.424142
C	-3.643793	4.330927	0.714829
C	-2.523049	3.807499	1.366811
C	-1.913055	2.647791	0.872742
O	-0.787672	2.095875	1.432813
C	-0.198020	2.736038	2.563732
H	-0.864828	2.686814	3.439904
H	0.731840	2.199127	2.778804
H	0.048995	3.786734	2.343125
H	-2.139944	4.308935	2.254273
H	-4.112650	5.235221	1.110262
H	-5.036159	4.129603	-0.931609
H	-3.977190	2.048372	-1.783504
C	-0.537293	0.961257	-2.250686
C	0.720606	0.090652	-2.360865
P	1.652044	0.087707	-0.740377
C	2.962021	-1.172400	-0.953074
C	3.023449	-2.068750	-2.028671
C	4.021243	-3.046767	-2.095921
C	4.973968	-3.130293	-1.080386
C	4.939648	-2.246774	0.004017
C	3.934955	-1.273995	0.071795
O	3.809829	-0.378051	1.085815
C	4.799730	-0.310622	2.100350
H	4.513239	0.519594	2.759365
H	4.841723	-1.241242	2.692325
H	5.795743	-0.101074	1.674805
H	5.691873	-2.324708	0.788662
H	5.759042	-3.889086	-1.124952
H	4.052136	-3.735808	-2.942407
H	2.291138	-2.010587	-2.834954
C	2.534711	1.703758	-0.815304
C	1.859693	2.856695	-0.380742
C	2.471296	4.111672	-0.463232
C	3.769597	4.226156	-0.967047
C	4.450563	3.081109	-1.395053
C	3.838238	1.827441	-1.324968
H	4.381174	0.943891	-1.668006
H	5.466259	3.164505	-1.790075
H	4.251753	5.205005	-1.026436
H	1.931010	5.000946	-0.128285
H	0.853061	2.773870	0.027522
H	0.452341	-0.950966	-2.592669
H	1.375768	0.455384	-3.166993
H	-0.266219	2.010572	-2.058995
H	-1.118424	0.950916	-3.185844
C	1.400928	-1.789155	2.662210
C	1.227886	-0.514877	3.051130
H	0.474333	-0.240919	3.795763
H	1.893816	0.269405	2.679185
H	0.784378	-2.601654	3.054299
H	2.193080	-2.064033	1.962701

^{4}9B-07

Geometry with 85 atoms:

Total energy: -3274.498004890

Cr	-0.664895	-0.611240	1.136266
C	-1.155102	-2.474079	0.399386
C	-2.586384	-3.012115	0.443699
C	-3.114445	-3.427583	1.827607
C	-3.759834	-2.337526	2.693307
C	-2.847739	-1.251673	3.275593
C	-2.329423	-0.210999	2.279009
H	-1.961645	0.680857	2.825329
H	-3.163536	0.138673	1.645962
H	-2.013465	-1.734686	3.819707
H	-3.426393	-0.728488	4.062281
H	-4.265367	-2.840938	3.536205
H	-4.564190	-1.850148	2.110703
H	-3.878012	-4.209655	1.675560
H	-2.302881	-3.919377	2.397934
H	-3.289433	-2.294057	-0.010224
H	-2.628623	-3.904516	-0.210957
H	-0.788846	-2.457870	-0.644430
H	-0.491081	-3.174445	0.939890
P	-1.557559	0.396227	-0.902252
C	-3.218456	-0.028588	-1.521003
C	-3.396314	-0.995922	-2.524148
C	-4.684298	-1.377941	-2.909764
C	-5.801652	-0.803496	-2.297830
C	-5.630220	0.163254	-1.300982
C	-4.346876	0.550351	-0.912088
H	-4.224903	1.311553	-0.137923
H	-6.500323	0.619607	-0.823008
H	-6.807380	-1.106322	-2.599105
H	-4.812387	-2.130275	-3.691760
H	-2.538185	-1.465300	-3.008073
C	-1.529915	2.219246	-0.755510
C	-2.089733	3.035661	-1.750984
C	-2.034767	4.426049	-1.656661
C	-1.410916	5.009143	-0.550901
C	-0.845842	4.219223	0.453282
C	-0.899598	2.820415	0.355046
O	-0.349200	1.990427	1.297652
C	0.097667	2.570575	2.526115
H	0.420989	1.745240	3.165359
H	0.954056	3.241210	2.361669
H	-0.722324	3.112619	3.023183
H	-0.366521	4.702115	1.303179
H	-1.361364	6.096873	-0.459675
H	-2.478488	5.048261	-2.436409
H	-2.586562	2.569978	-2.605819
C	-0.370065	0.061691	-2.291815
C	1.036808	0.535211	-1.911737
P	1.604029	-0.254375	-0.311294
C	2.666309	-1.646829	-0.849770
C	2.347492	-2.962111	-0.482991
C	3.159463	-4.037283	-0.856048
C	4.311987	-3.793096	-1.604011
C	4.654806	-2.493118	-1.989260
C	3.833813	-1.415888	-1.625142
O	4.076257	-0.133305	-1.971473
C	5.299604	0.221973	-2.595737
H	6.165341	-0.068163	-1.976190
H	5.395528	-0.232897	-3.596855
H	5.283471	1.315065	-2.699461
H	5.556878	-2.327059	-2.578170
H	4.959361	-4.622645	-1.899600
H	2.892351	-5.054356	-0.562212
H	1.444973	-3.150094	0.098021
C	2.780944	0.928904	0.464991
C	2.678635	2.319809	0.303733
C	3.545792	3.178501	0.986667
C	4.517914	2.663715	1.849216
C	4.620114	1.279663	2.023623
C	3.759039	0.419121	1.338216
H	3.864698	-0.660689	1.473457
H	5.378964	0.865148	2.692077
H	5.195329	3.336944	2.380024
H	3.459509	4.258174	0.838910
H	1.925421	2.754755	-0.355229
H	1.763333	0.299906	-2.700858
H	1.045377	1.627549	-1.788301
H	-0.723953	0.566104	-3.205066
H	-0.379678	-1.023246	-2.483204
C	0.798934	-0.845228	3.416229
C	0.749604	-2.121025	3.003523
H	1.521232	-2.538823	2.350193
H	-0.033147	-2.805493	3.341897
H	1.622992	-0.186880	3.120424
H	0.058772	-0.447221	4.116803

^{4}9B-08

Geometry with 85 atoms:

Total energy: -3274.497355160

Cr	-0.408998	-0.312724	1.177491
C	-0.392094	-2.306607	0.618873
C	-0.802646	-3.335889	1.673767
C	-2.302620	-3.649782	1.751011
C	-3.251163	-2.449652	1.885504
C	-2.839238	-1.395112	2.932619
C	-2.135608	-0.168724	2.344398
H	-1.848362	0.534805	3.149761
H	-2.859076	0.386732	1.718730
H	-2.211615	-1.870237	3.708675
H	-3.742831	-1.055942	3.473994
H	-4.254814	-2.841408	2.121162
H	-3.355286	-1.953937	0.909351
H	-2.591771	-4.218563	0.848484
H	-2.463276	-4.334976	2.603044
H	-0.276712	-4.289452	1.473365
H	-0.439900	-3.034112	2.672405
H	-0.980477	-2.457688	-0.304712
H	0.666432	-2.453202	0.342373
P	-1.641991	0.337271	-0.830329
C	-3.243846	-0.435728	-1.234420
C	-3.279056	-1.633070	-1.970751
C	-4.490358	-2.299603	-2.170939
C	-5.674790	-1.781864	-1.638837
C	-5.646611	-0.589349	-0.909029
C	-4.439218	0.081034	-0.703631
H	-4.430050	1.007935	-0.127010
H	-6.569351	-0.178841	-0.492265
H	-6.620246	-2.307075	-1.794189
H	-4.506191	-3.229353	-2.744580
H	-2.366342	-2.060244	-2.389671
C	-1.954198	2.134881	-0.709388
C	-2.733743	2.805271	-1.665846
C	-2.965271	4.177119	-1.572826
C	-2.412408	4.890122	-0.506370
C	-1.626960	4.248516	0.454301
C	-1.384835	2.871329	0.350060
O	-0.588321	2.192273	1.246338
C	-0.222869	2.864502	2.454904
H	0.379612	2.160353	3.036719
H	0.385282	3.757803	2.246034
H	-1.116964	3.146722	3.032762
H	-1.207247	4.831958	1.272117
H	-2.591009	5.964081	-0.413599
H	-3.577651	4.683491	-2.321588
H	-3.180396	2.236308	-2.485209
C	-0.603434	0.185536	-2.359955
C	0.764574	0.837700	-2.137658
P	1.647860	0.160502	-0.639695
C	2.506122	-1.336195	-1.276409
C	2.228342	-1.927976	-2.516454
C	2.881777	-3.094861	-2.926624
C	3.834336	-3.679398	-2.092136
C	4.137829	-3.109680	-0.851632
C	3.470787	-1.949232	-0.439065
O	3.691574	-1.330396	0.745981
C	4.719272	-1.783810	1.610686
H	4.731494	-1.094339	2.465321
H	4.524753	-2.807115	1.976174
H	5.704036	-1.753553	1.113920
H	4.889790	-3.574214	-0.213935
H	4.355185	-4.588044	-2.403816
H	2.648876	-3.537622	-3.897220
H	1.497752	-1.479978	-3.191093
C	2.997883	1.388388	-0.415031
C	4.136072	1.403642	-1.237617
C	5.123165	2.374331	-1.051281
C	4.985377	3.336746	-0.044280
C	3.856298	3.324902	0.779432
C	2.868901	2.352316	0.595423

H	1.990513	2.340338	1.239716
H	3.745873	4.071286	1.570493
H	5.760626	4.093562	0.098965
H	6.006261	2.379514	-1.695257
H	4.256440	0.650511	-2.020356
H	1.402395	0.745628	-3.030410
H	0.649896	1.916447	-1.944170
H	-1.137455	0.648601	-3.204712
H	-0.498728	-0.887529	-2.579430
C	0.580644	-0.594242	3.675585
C	1.592547	-0.713974	2.798917
H	2.256732	0.121094	2.556235
H	1.843469	-1.672947	2.341968
H	0.368942	0.345232	4.194158
H	-0.034478	-1.447780	3.967529

^{4}9B-09
Geometry with 85 atoms:
Total energy: -3274.498526540

Cr	-0.305096	-0.426777	1.136909
C	-0.283704	-2.387203	0.460896
C	-0.725642	-3.508071	1.402368
C	-2.232852	-3.778400	1.484377
C	-3.125350	-2.582968	1.852968
C	-2.583814	-1.687269	2.985819
C	-1.874342	-0.422883	2.493606
H	-1.426208	0.122066	3.349647
H	-2.623170	0.264958	2.055596
H	-1.914334	-2.276934	3.638308
H	-3.423510	-1.390287	3.642467
H	-4.120113	-2.975297	2.122733
H	-3.289921	-1.960389	0.962217
H	-2.578646	-4.189655	0.518571
H	-2.386540	-4.583274	2.225721
H	-0.239440	-4.450739	1.082943
H	-0.336343	-3.330918	2.419492
H	-0.836917	-2.458000	-0.494145
H	0.785219	-2.508629	0.213846
P	-1.662812	0.324446	-0.766023
C	-3.290316	-0.417182	-1.120166
C	-3.384662	-1.593395	-1.884213
C	-4.619451	-2.226561	-2.046910
C	-5.766402	-1.697130	-1.448014
C	-5.678056	-0.525845	-0.688979
C	-4.447602	0.112353	-0.522512
H	-4.390576	1.024743	0.074826
H	-6.571592	-0.107020	-0.220002
H	-6.729830	-2.196892	-1.574021
H	-4.683133	-3.139903	-2.643168
H	-2.500537	-2.029374	-2.353108
C	-1.951477	2.128812	-0.658263
C	-2.655274	2.799546	-1.672758
C	-2.842911	4.179982	-1.627856
C	-2.318383	4.904896	-0.554078
C	-1.617191	4.261811	0.467487
C	-1.429931	2.871954	0.419288
O	-0.736839	2.191489	1.391924
C	-0.593006	2.825231	2.666462
H	-0.248823	2.059169	3.367368
H	0.148030	3.639972	2.628142
H	-1.559870	3.215313	3.020203
H	-1.215758	4.850427	1.291251
H	-2.455345	5.987781	-0.504530
H	-3.396045	4.685837	-2.421732
H	-3.075121	2.224531	-2.502111
C	-0.682958	0.181279	-2.338890
C	0.676604	0.869180	-2.170569
P	1.608769	0.199263	-0.701452
C	2.517183	-1.252934	-1.360632
C	2.318192	-1.779417	-2.644612
C	2.994880	-2.926616	-3.070670
C	3.889345	-3.557964	-2.206549
C	4.108863	-3.056586	-0.919717
C	3.417487	-1.916426	-0.491342
O	3.553093	-1.370502	0.744538
C	4.557218	-1.852206	1.625794
H	4.373356	-2.899109	1.921814
H	5.559237	-1.770179	1.171651
H	4.516245	-1.216904	2.519865
H	4.812709	-3.561172	-0.258464
H	4.428205	-4.451909	-2.529793
H	2.825392	-3.317753	-4.075932
H	1.630182	-1.295322	-3.338657
C	2.888210	1.482631	-0.405933
C	4.180078	1.421181	-0.951401
C	5.100632	2.439280	-0.687677
C	4.741203	3.525975	0.116570
C	3.455186	3.592967	0.661998
C	2.535111	2.572830	0.407561
H	1.534410	2.617306	0.841284
H	3.169982	4.439322	1.292196
H	5.464497	4.319581	0.319590
H	6.105110	2.383884	-1.114810
H	4.471207	0.577860	-1.581702
H	1.284332	0.798109	-3.085486
H	0.543445	1.944688	-1.971594
H	-1.259898	0.628649	-3.163351
H	-0.560717	-0.890002	-2.560382
C	1.297404	-1.318367	3.080361
C	1.704625	-0.051133	2.896029
H	1.308860	0.762642	3.509378
H	2.495930	0.201198	2.187113
H	0.550331	-1.577155	3.835991
H	1.745256	-2.140206	2.516320

^{4}9B-10
Geometry with 85 atoms:
Total energy: -3274.496944140

Cr	-0.423601	-0.532759	1.129090
C	-0.715222	-2.477612	0.567168
C	-2.078832	-3.141435	0.386452
C	-2.872583	-3.463361	1.659272
C	-3.616334	-2.309982	2.345906
C	-2.776260	-1.308433	3.150064
C	-2.064261	-0.217479	2.350191
H	-1.652566	0.539818	3.045864
H	-2.811154	0.320571	1.739411
H	-2.060862	-1.869919	3.778401
H	-3.456307	-0.813647	3.871312
H	-4.347618	-2.761572	3.038676
H	-4.216265	-1.765056	1.593121
H	-3.627181	-4.223443	1.391650
H	-2.206391	-3.956092	2.393681
H	-2.720398	-2.545162	-0.282636
H	-1.920868	-4.098448	-0.149824
H	-0.130444	-2.543024	-0.368144
H	-0.128144	-3.029435	1.324306
P	-1.548184	0.316681	-0.870108
C	-3.236209	-0.152147	-1.379136
C	-3.446517	-1.102629	-2.392770
C	-4.743698	-1.508169	-2.718099
C	-5.839721	-0.973787	-2.035306
C	-5.636802	-0.025785	-1.026727
C	-4.343606	0.383964	-0.697334
H	-4.200083	1.131294	0.086202
H	-6.490175	0.398257	-0.492211
H	-6.852934	-1.293967	-2.289826
H	-4.895600	-2.247030	-3.508596
H	-2.604323	-1.542248	-2.929793
C	-1.589756	2.138519	-0.690258
C	-2.253877	2.953705	-1.620914
C	-2.263802	4.341540	-1.483562
C	-1.602952	4.923962	-0.398737
C	-0.934593	4.135786	0.541183
C	-0.922171	2.741193	0.396965
O	-0.257785	1.914548	1.271559
C	0.256680	2.479116	2.483636
H	0.632806	1.645537	3.084608
H	1.085542	3.170698	2.272840
H	-0.540291	2.991518	3.044422
H	-0.422291	4.617651	1.371888
H	-1.604548	6.009446	-0.274166
H	-2.786577	4.962859	-2.213438
H	-2.782460	2.487517	-2.456302
C	-0.469439	0.033164	-2.353622
C	0.915948	0.648868	-2.134224
P	1.738324	0.025302	-0.563785
C	3.050492	-1.098963	-1.223351
C	3.958118	-0.587095	-2.168450
C	4.966629	-1.375804	-2.719055
C	5.080998	-2.709228	-2.317011
C	4.206885	-3.242775	-1.370263
C	3.192730	-2.444096	-0.810280
O	2.336537	-2.901242	0.135170
C	2.379574	-4.264460	0.529315
H	2.194235	-4.937775	-0.324742
H	3.344480	-4.522087	0.998648
H	1.576883	-4.398712	1.265086
H	4.321800	-4.281792	-1.064208
H	5.863746	-3.345274	-2.737839
H	5.657914	-0.952794	-3.450801
H	3.878909	0.460203	-2.472069
C	2.754985	1.447112	0.031826
C	2.408478	2.789997	-0.189043
C	3.165446	3.823070	0.373817
C	4.273381	3.532627	1.174310
C	4.625380	2.198133	1.404303
C	3.875918	1.165625	0.836726
H	4.175878	0.129275	1.010955
H	5.494485	1.958120	2.021927
H	4.864119	4.340864	1.612085
H	2.883124	4.861374	0.181402
H	1.539742	3.055214	-0.792332
H	1.565394	0.434819	-2.994727
H	0.825397	1.741639	-2.066723
H	-0.951782	0.464771	-3.245018
H	-0.402241	-1.057002	-2.503464
C	1.662164	-0.963012	2.698912
C	0.622399	-1.278878	3.491520
H	0.191921	-2.283440	3.498685
H	0.203092	-0.568936	4.209906
H	2.114837	-1.700891	2.031166
H	2.144074	0.018821	2.746458

^{4}9B-11
Geometry with 85 atoms:
Total energy: -3274.497747700

Cr	-0.293074	0.056835	1.128392
C	-0.377195	-1.995981	1.067977
C	-1.623517	-2.751277	1.522534
C	-1.938740	-2.711426	3.029456
C	-2.831427	-1.566998	3.531400
C	-2.230549	-0.157374	3.595517
C	-1.966980	0.523251	2.248949
H	-1.786960	1.606713	2.402826
H	-2.883259	0.454870	1.638766
H	-1.317501	-0.186361	4.219206
H	-2.938720	0.468918	4.173465
H	-3.169820	-1.831072	4.548968
H	-3.747512	-1.536912	2.912059
H	-2.451117	-3.652791	3.291708
H	-0.993337	-2.724895	3.605452
H	-2.509088	-2.410735	0.959834
H	-1.495583	-3.813343	1.234379
H	-0.149367	-2.245969	0.014313
H	0.504411	-2.324709	1.647616
P	-1.596897	0.237712	-0.933529
C	-2.992953	-0.893179	-1.244562
C	-2.814917	-2.056115	-2.014244
C	-3.844886	-2.994247	-2.123038
C	-5.060115	-2.786405	-1.465484
C	-5.245285	-1.631360	-0.698772
C	-4.219830	-0.691484	-0.584147
H	-4.378515	0.199890	0.025153
H	-6.192624	-1.461020	-0.181673
H	-5.862364	-3.523463	-1.549381
H	-3.691937	-3.893964	-2.723700
H	-1.872090	-2.251057	-2.528263
C	-2.253630	1.947024	-0.952953
C	-3.418195	2.322033	-1.637288
C	-3.890641	3.635416	-1.580872
C	-3.195015	4.583361	-0.828677
C	-2.022729	4.237394	-0.148559
C	-1.545324	2.924604	-0.220428
O	-0.379293	2.517704	0.392037
C	0.538617	3.518610	0.841995
H	1.493641	3.014102	1.019737
H	0.691784	4.285318	0.066725
H	0.185886	3.992791	1.771896
H	-1.498474	4.993484	0.434962
H	-3.562699	5.610227	-0.764606
H	-4.800407	3.912789	-2.117225
H	-3.967588	1.574336	-2.213039

C	-0.481949	0.157916	-2.418250
C	0.830769	0.899366	-2.132648
P	1.714250	0.167678	-0.664957
C	2.438659	-1.393229	-1.336857
C	2.456868	-1.682065	-2.710376
C	2.943210	-2.897388	-3.198651
C	3.427443	-3.848894	-2.301927
C	3.435620	-3.587448	-0.930031
C	2.950790	-2.364800	-0.442219
O	2.957916	-2.042175	0.877865
C	3.389852	-3.006922	1.827665
H	3.274177	-2.547311	2.817855
H	2.772447	-3.919876	1.786324
H	4.451297	-3.269990	1.682890
H	3.828299	-4.339676	-0.247560
H	3.810235	-4.805602	-2.665504
H	2.943113	-3.093472	-4.272870
H	2.085197	-0.951775	-3.429704
C	3.144334	1.296775	-0.392653
C	3.410485	2.410939	-1.207724
C	4.468418	3.274104	-0.903286
C	5.276726	3.036077	0.211358
C	5.025774	1.924458	1.022521
C	3.966542	1.063754	0.726827
H	3.784982	0.194251	1.359933
H	5.657348	1.725643	1.891975
H	6.102753	3.712015	0.445228
H	4.663205	4.135463	-1.547247
H	2.802895	2.622865	-2.088772
H	1.470200	0.917822	-3.027286
H	0.623168	1.946883	-1.869986
H	-1.005281	0.588626	-3.286106
H	-0.288409	-0.902697	-2.637992
C	1.307981	-0.286733	3.215075
C	1.126053	1.041537	3.153357
H	0.332593	1.545905	3.712227
H	1.825916	1.669934	2.596390
H	0.668513	-0.932649	3.822049
H	2.129508	-0.762399	2.679730

^{4}9B-12
Geometry with 85 atoms:
Total energy: -3274.497296950

Cr	-0.357844	-0.299796	1.375819
C	-0.706095	-2.317146	1.429675
C	-1.999029	-2.953681	0.924668
C	-3.185584	-2.929783	1.896016
C	-3.800092	-1.569622	2.255506
C	-2.962520	-0.635274	3.150464
C	-2.025512	0.331753	2.426946
H	-1.585151	1.046818	3.149170
H	-2.616588	0.955345	1.732067
H	-2.405409	-1.246237	3.884935
H	-3.666781	-0.035166	3.759317
H	-4.748179	-1.779167	2.779875
H	-4.085577	-1.037107	1.332236
H	-3.986629	-3.553517	1.461057
H	-2.884805	-3.440934	2.830674
H	-2.315058	-2.505879	-0.032891
H	-1.802136	-4.018213	0.687297
H	0.156357	-2.678722	0.846221
H	-0.537811	-2.618411	2.479652
P	-1.411503	0.252087	-0.780613
C	-3.175167	-0.010194	-1.178999
C	-3.590259	-1.137231	-1.908928
C	-4.950164	-1.371498	-2.129893
C	-5.907222	-0.485151	-1.628358
C	-5.500365	0.644174	-0.910311
C	-4.143543	0.882258	-0.684839
H	-3.839669	1.769767	-0.125656
H	-6.243274	1.344472	-0.521160
H	-6.969968	-0.671663	-1.800714
H	-5.260808	-2.251568	-2.698083
H	-2.860865	-1.843594	-2.308886
C	-1.169016	2.060537	-0.948896
C	-1.654729	2.748383	-2.073305
C	-1.457447	4.120537	-2.219606
C	-0.770981	4.818874	-1.222215
C	-0.277319	4.159089	-0.095109
C	-0.467022	2.776095	0.042440
O	0.025403	2.066092	1.112460
C	0.703561	2.784589	2.149429
H	0.984938	2.051238	2.910355
H	1.613261	3.264432	1.759847
H	0.035488	3.532160	2.604850
H	0.263568	4.728923	0.657683
H	-0.612085	5.895744	-1.317407
H	-1.841092	4.641598	-3.099027
H	-2.207252	2.195899	-2.837769
C	-0.465295	-0.454917	-2.209149
C	1.004450	-0.027284	-2.169670
P	1.803064	-0.253091	-0.479639
C	3.031761	-1.598696	-0.786892
C	4.423381	-1.437519	-0.729583
C	5.287344	-2.519605	-0.926632
C	4.761397	-3.784248	-1.189041
C	3.378710	-3.970743	-1.280507
C	2.517201	-2.882266	-1.094448
O	1.166260	-2.961381	-1.216214
C	0.543897	-4.215705	-1.450293
H	0.860448	-4.648979	-2.414444
H	0.756760	-4.930267	-0.637258
H	-0.536328	-4.025221	-1.479101
H	2.981430	-4.960400	-1.503631
H	5.426886	-4.638289	-1.336610
H	6.367497	-2.367005	-0.876654
H	4.851631	-0.453764	-0.537591
C	2.824824	1.257971	-0.189930
C	2.671066	2.451708	-0.913080
C	3.389428	3.600699	-0.563886
C	4.276350	3.581558	0.514473
C	4.438890	2.400650	1.247136
C	3.716901	1.256614	0.903066
H	3.870920	0.344667	1.483317
H	5.133118	2.367775	2.090571
H	4.839801	4.478639	0.782208
H	3.247579	4.516014	-1.143609
H	1.978378	2.516165	-1.751744
H	1.588993	-0.599766	-2.903657
H	1.086827	1.029817	-2.453638
H	-0.939267	-0.136782	-3.151029
H	-0.548941	-1.547759	-2.136129
C	1.579105	-0.702361	3.069142
C	0.543087	-0.516115	3.905673
H	-0.123319	-1.331168	4.195975
H	0.355961	0.450903	4.381684
H	1.817377	-1.685976	2.653831
H	2.277361	0.108953	2.851630

^{4}9B-13
Geometry with 85 atoms:
Total energy: -3274.496322970

Cr	-0.712637	-0.547634	1.212996
C	-1.050972	-2.503472	0.648534
C	-2.404500	-3.197973	0.804183
C	-2.936705	-3.215633	2.252129
C	-4.010944	-2.163588	2.574249
C	-3.795946	-0.769275	1.975207
C	-2.450459	-0.106137	2.271829
H	-2.198933	-0.226903	3.343156
H	-2.533628	0.984106	2.101859
H	-4.616353	-0.123910	2.345422
H	-3.957538	-0.823067	0.888183
H	-4.105179	-2.081163	3.672439
H	-4.988900	-2.533315	2.217171
H	-3.354469	-4.208857	2.486616
H	-2.083048	-3.095330	2.940785
H	-3.150890	-2.737865	0.133655
H	-2.303759	-4.239896	0.444927
H	-0.677234	-2.610895	-0.386689
H	-0.311006	-3.012518	1.299539
P	-1.560707	0.325456	-0.884780
C	-3.215778	-0.071138	-1.538625
C	-3.401323	-1.256386	-2.272528
C	-4.678789	-1.619730	-2.705892
C	-5.779569	-0.811184	-2.407055
C	-5.601100	0.364546	-1.671372
C	-4.327506	0.733538	-1.233985
H	-4.202939	1.646338	-0.648396
H	-6.458788	0.997208	-1.430718
H	-6.777734	-1.098666	-2.746066
H	-4.813471	-2.541548	-3.276684
H	-2.556887	-1.908890	-2.504268
C	-1.459553	2.147375	-0.742818
C	-1.938639	2.994644	-1.755041
C	-1.822835	4.380419	-1.648164
C	-1.218760	4.929071	-0.513971
C	-0.724871	4.108515	0.503049
C	-0.834810	2.715591	0.388004
O	-0.325267	1.855765	1.333454
C	0.122834	2.399663	2.581152
H	0.400997	1.550147	3.211954
H	1.007725	3.037141	2.437674
H	-0.685612	2.962930	3.072383
H	-0.251746	4.562899	1.371844
H	-1.124940	6.012932	-0.412551
H	-2.204369	5.026745	-2.441086
H	-2.421376	2.557656	-2.632646
C	-0.370882	-0.049609	-2.262814
C	1.036131	0.432917	-1.905764
P	1.613455	-0.264575	-0.266401
C	2.661409	-1.698360	-0.728633
C	2.369131	-2.976628	-0.231528
C	3.166005	-4.081140	-0.546108
C	4.278536	-3.906081	-1.369606
C	4.598597	-2.644565	-1.880815
C	3.795440	-1.537407	-1.569691
O	4.030561	-0.288438	-2.026897
C	5.218729	0.000100	-2.746520
H	5.207018	1.081838	-2.934914
H	6.116891	-0.252846	-2.157432
H	5.251203	-0.533582	-3.712212
H	5.471294	-2.532165	-2.523898
H	4.912552	-4.759220	-1.624180
H	2.917215	-5.067058	-0.148422
H	1.498492	-3.113386	0.408316
C	2.819664	0.966293	0.386020
C	2.638800	2.348795	0.216940
C	3.520285	3.259186	0.808527
C	4.590907	2.804678	1.583775
C	4.778726	1.429638	1.758147
C	3.902295	0.518111	1.164548
H	4.073464	-0.552767	1.298149
H	5.617330	1.061830	2.354829
H	5.279492	3.517149	2.044349
H	3.367807	4.330959	0.656507
H	1.811948	2.737784	-0.379166
H	1.760519	0.156606	-2.683034
H	1.051831	1.529678	-1.832791
H	-0.732444	0.433511	-3.184562
H	-0.385317	-1.137829	-2.431852
C	1.356912	-1.110937	2.986495
C	0.254991	-1.240652	3.742914
H	-0.279671	-2.190279	3.828033
H	-0.119296	-0.416499	4.357492
H	1.775452	-1.956608	2.433629
H	1.931304	-0.180137	2.957392

^{4}9B-14
Geometry with 85 atoms:
Total energy: -3274.497267220

Cr	-0.416744	-0.872867	1.005104
C	-0.697189	-2.659124	0.035544
C	-2.055104	-3.285309	-0.277384
C	-2.843644	-3.883337	0.895101
C	-3.642092	-2.912078	1.774452
C	-2.852640	-2.046589	2.763442
C	-2.125025	-0.832962	2.184042
H	-1.786053	-0.187664	3.016510
H	-2.854027	-0.225108	1.616342
H	-2.158840	-2.696574	3.326952
H	-3.571939	-1.680379	3.522543
H	-4.360657	-3.513231	2.358736
H	-4.256305	-2.258140	1.127498
H	-3.562755	-4.607598	0.474349
H	-2.163024	-4.481130	1.531888
H	-2.704562	-2.562609	-0.797592
H	-1.891099	-4.100165	-1.011090
H	-0.138504	-2.505400	-0.903619
H	-0.084677	-3.360172	0.634454
P	-1.397320	0.412112	-0.832593
C	-3.140227	0.188127	-1.348280
C	-3.487600	-0.706265	-2.375420

C	-4.829963	-0.944622	-2.680611
C	-5.840182	-0.302345	-1.959288
C	-5.502959	0.583418	-0.931137
C	-4.162724	0.828561	-0.624705
H	-3.915594	1.525451	0.178381
H	-6.287274	1.088767	-0.362545
H	-6.889544	-0.491856	-2.197648
H	-5.084868	-1.639844	-3.483951
H	-2.718500	-1.237110	-2.939635
C	-1.299397	2.153573	-0.272471
C	-1.784831	3.194903	-1.079780
C	-1.711795	4.523237	-0.664839
C	-1.150336	4.816616	0.580714
C	-0.663059	3.799957	1.403606
C	-0.728292	2.465990	0.978219
O	-0.233684	1.428621	1.735052
C	0.148568	1.698430	3.086740
H	0.480255	0.747553	3.516836
H	0.979319	2.417120	3.125795
H	-0.707170	2.079293	3.665448
H	-0.221909	4.058945	2.364057
H	-1.086818	5.851935	0.923853
H	-2.095383	5.321574	-1.303309
H	-2.239610	2.954035	-2.044142
C	-0.378361	0.372675	-2.404769
C	1.046505	-0.189072	-2.237138
P	1.753085	-0.063845	-0.520619
C	3.406420	-0.867014	-0.697298
C	4.607502	-0.140570	-0.702133
C	5.843271	-0.783241	-0.817020
C	5.888759	-2.172820	-0.932596
C	4.709592	-2.923097	-0.940895
C	3.471244	-2.276102	-0.826800
O	2.279162	-2.923997	-0.836401
C	2.236634	-4.334821	-0.993884
H	1.175397	-4.611772	-1.000662
H	2.698356	-4.647495	-1.945831
H	2.738454	-4.850118	-0.156896
H	4.762574	-4.007066	-1.037921
H	6.848950	-2.686795	-1.022264
H	6.763684	-0.195569	-0.819366
H	4.583595	0.946445	-0.617709
C	2.195226	1.701178	-0.273729
C	2.019985	2.692761	-1.250009
C	2.349308	4.024625	-0.975272
C	2.871411	4.378973	0.270348
C	3.061423	3.395024	1.247831
C	2.716645	2.070009	0.979916
H	2.862360	1.309897	1.752293
H	3.477784	3.662680	2.222326
H	3.131492	5.419177	0.480519
H	2.198664	4.786395	-1.743818
H	1.628338	2.443203	-2.236459
H	1.058011	-1.272179	-2.430199
H	1.738123	0.267728	-2.961096
H	-0.362730	1.404569	-2.783906
H	-0.924716	-0.222647	-3.148999
C	1.610672	-1.706648	2.420510
C	0.526131	-2.073992	3.128590
H	0.008920	-3.015947	2.932401
H	0.157951	-1.488452	3.975919
H	2.011694	-2.336050	1.621589
H	2.180954	-0.804191	2.664851

^{4}9B-15

Geometry with 85 atoms:

Total energy: -3274.497636090

Cr	-0.396858	-0.423299	1.354830
C	-0.545535	-2.449525	1.042259
C	-1.695476	-3.041736	0.224631
C	-2.986452	-3.325231	1.003088
C	-3.709956	-2.141919	1.661010
C	-2.994038	-1.468991	2.849589
C	-2.106048	-0.272148	2.504982
H	-1.699278	0.159550	3.442556
H	-2.723984	0.525923	2.052245
H	-2.415112	-2.231023	3.402881
H	-3.769772	-1.127946	3.562595
H	-4.682932	-2.522514	2.015870
H	-3.951430	-1.381050	0.900448
H	-3.696608	-3.816168	0.313691
H	-2.762370	-4.074971	1.785412
H	-1.936325	-2.408613	-0.646554
H	-1.368713	-4.003224	-0.216168
H	0.428349	-2.713998	0.598742
H	-0.561772	-2.887580	2.054982
P	-1.438302	0.392282	-0.709872
C	-3.216338	0.282402	-1.101714
C	-3.715987	-0.696260	-1.977029
C	-5.093463	-0.817627	-2.180450
C	-5.980624	0.033331	-1.515540
C	-5.487497	1.015547	-0.649586
C	-4.113364	1.140833	-0.441296
H	-3.737916	1.911710	0.235907
H	-6.176969	1.687350	-0.132757
H	-7.057037	-0.065774	-1.674809
H	-5.473404	-1.581530	-2.863004
H	-3.039955	-1.373199	-2.502315
C	-1.066012	2.186694	-0.707644
C	-1.264687	2.972737	-1.854316
C	-0.948021	4.330278	-1.856917
C	-0.426920	4.913808	-0.698032
C	-0.225960	4.154389	0.455846
C	-0.543654	2.790022	0.451136
O	-0.352193	1.988037	1.558269
C	-0.328357	2.624695	2.842440
H	-0.402394	1.831500	3.593449
H	0.607855	3.184616	2.994042
H	-1.189147	3.301963	2.952508
H	0.189842	4.627816	1.344070
H	-0.170054	5.975645	-0.686719
H	-1.108527	4.930476	-2.754736
H	-1.681445	2.511178	-2.753313
C	-0.533424	-0.237768	-2.200126
C	0.954313	0.118565	-2.132080
P	1.691021	-0.122776	-0.417928
C	2.824120	-1.569705	-0.509370
C	4.062452	-1.534753	0.152599
C	4.895571	-2.655631	0.195891
C	4.491681	-3.834363	-0.432138
C	3.264296	-3.899181	-1.097690
C	2.426393	-2.775385	-1.135705
O	1.216911	-2.763085	-1.753267
C	0.720535	-3.945475	-2.358645
H	0.615121	-4.763296	-1.626440
H	-0.270951	-3.697510	-2.759703
H	1.367083	-4.277599	-3.189014
H	2.967412	-4.827427	-1.585090
H	5.134276	-4.717973	-0.410959
H	5.855738	-2.602207	0.713185
H	4.389747	-0.610790	0.633984
C	2.864794	1.292109	-0.314781
C	3.792205	1.533921	-1.345494
C	4.663394	2.621350	-1.269322
C	4.624985	3.477526	-0.161615
C	3.710994	3.242187	0.867604
C	2.834142	2.154766	0.789554
H	2.114784	1.979834	1.587107
H	3.678052	3.906491	1.734956
H	5.310650	4.326456	-0.103016
H	5.379488	2.800470	-2.075119
H	3.840640	0.864151	-2.207997
H	1.522986	-0.463820	-2.869214
H	1.097053	1.184910	-2.360178
H	-0.996305	0.168603	-3.112834
H	-0.669043	-1.327186	-2.206893
C	1.681686	-0.342679	3.123816
C	0.926011	-1.329603	3.632058
H	1.129395	-2.376371	3.392647
H	0.116927	-1.135744	4.342305
H	2.536070	-0.555337	2.475107
H	1.541515	0.698108	3.427136

^{4}9B-16

Geometry with 85 atoms:

Total energy: -3274.492625320

Cr	-0.063673	0.133311	-1.406172
P	1.412053	0.387254	0.729857
P	-1.906982	0.409838	0.528683
O	4.036676	-0.163092	-0.406525
O	-1.721284	-2.469737	0.920854
C	-1.477608	-0.499445	-2.746507
C	-1.116434	-1.844391	-2.178137
C	-0.466647	-2.868783	-3.124078
C	1.028270	-2.666850	-3.404950
C	1.449529	-1.244762	-3.807392
C	1.576863	-0.272502	-2.631683
H	1.918971	0.716751	-2.986801
H	2.361648	-0.637037	-1.950533
H	0.758007	-0.858622	-4.577508
H	2.432107	-1.315929	-4.312831
H	1.319844	-3.378922	-4.194826
H	1.609770	-2.959030	-2.509770
H	-0.610620	-3.878885	-2.704663
H	-1.029236	-2.848135	-4.072417
H	-0.375664	-1.741879	-1.288260
H	-1.971689	-2.283124	-1.644595
H	-2.511115	-0.186036	-2.553301
H	-1.209800	-0.349569	-3.798297
C	2.074201	-1.155321	1.485394
C	2.707770	-1.130722	2.738166
C	3.225068	-2.305529	3.289400
C	3.122639	-3.513901	2.591403
C	2.504949	-3.542363	1.337539
C	1.982547	-2.368186	0.787316
H	1.520842	-2.398206	-0.201660
H	2.433926	-4.481066	0.782020
H	3.531649	-4.431117	3.022215
H	3.716405	-2.276419	4.265073
H	2.816318	-0.188911	3.282867
C	2.842028	1.541771	0.675738
C	2.778422	2.856501	1.160908
C	3.863482	3.729658	1.035681
C	5.033670	3.286911	0.418317
C	5.127248	1.982748	-0.076038
C	4.036831	1.109894	0.044395
C	5.172837	-0.701770	-1.059155
H	4.915005	-1.738074	-1.315161
H	5.409308	-0.149049	-1.984712
H	6.055220	-0.705875	-0.396298
H	6.048646	1.651938	-0.554820
H	5.889138	3.959221	0.316562
H	3.790904	4.747927	1.423199
H	1.873219	3.220219	1.648694
C	0.328690	1.083899	2.076624
C	-1.003515	0.333233	2.151203
C	-3.319088	-0.747728	0.740050
C	-4.659106	-0.334407	0.719638
C	-5.702611	-1.259768	0.813742
C	-5.409409	-2.618427	0.930508
C	-4.082721	-3.058776	0.966139
C	-3.037493	-2.129641	0.876734
C	-1.355416	-3.837261	1.023780
H	-1.746318	-4.291078	1.950296
H	-1.712161	-4.418739	0.155940
H	-0.260068	-3.862197	1.053840
H	-3.873066	-4.123207	1.066600
H	-6.216602	-3.351790	0.999931
H	-6.738580	-0.915070	0.796139
H	-4.897633	0.726251	0.630086
C	-2.681826	2.075426	0.471829
C	-3.362013	2.436899	-0.707732
C	-3.936440	3.701978	-0.841160
C	-3.826052	4.634666	0.196176
C	-3.152547	4.287762	1.369841
C	-2.588328	3.015081	1.511780
H	-2.081845	2.768976	2.446562
H	-3.069548	5.008249	2.187401
H	-4.267414	5.628518	0.089893
H	-4.469136	3.962122	-1.759164
H	-3.456994	1.714883	-1.522628
H	-0.839767	-0.737110	2.344451
H	-1.639152	0.714542	2.964894
H	0.154671	2.145529	1.847552
H	0.860057	1.044115	3.039650
C	-0.473533	2.236393	-2.697002
C	0.213745	2.550393	-1.572938
H	1.307340	2.565942	-1.554295
H	-0.305647	2.947819	-0.695196
H	0.036790	1.956572	-3.621534
H	-1.556812	2.356229	-2.752389

^{4}9B-17

Geometry with 85 atoms:
Total energy: -3274.490361960

Cr	-0.157663	-0.409196	1.266792
P	-1.636676	0.233467	-0.792518
P	1.728854	0.560879	-0.536093
O	-3.729039	0.801109	1.080415
O	3.987808	-0.731320	0.708134
C	1.272774	-1.377558	2.369756
C	1.034265	-2.460917	1.357013
C	0.450106	-3.795003	1.851928
C	-1.055297	-3.801149	2.147214
C	-1.563523	-2.646276	3.022270
C	-1.738979	-1.316391	2.285510
H	-2.082070	-0.539531	2.990598
H	-2.529978	-1.420610	1.524086
H	-0.902903	-2.531078	3.900021
H	-2.545269	-2.945452	3.437562
H	-1.299634	-4.764813	2.624414
H	-1.616493	-3.787500	1.195191
H	0.665493	-4.573354	1.100651
H	1.008641	-4.080122	2.759436
H	0.298902	-2.103511	0.528238
H	1.926551	-2.629268	0.736534
H	2.261853	-0.914240	2.316961
H	0.981860	-1.623526	3.396184
C	-2.838505	-1.024623	-1.371580
C	-2.447860	-2.373066	-1.317029
C	-3.308247	-3.377682	-1.765470
C	-4.573188	-3.043695	-2.260155
C	-4.969550	-1.703610	-2.311405
C	-4.107091	-0.695248	-1.871835
H	-4.425326	0.348273	-1.921206
H	-5.956853	-1.439186	-2.698318
H	-5.251225	-3.828644	-2.603996
H	-2.993670	-4.423086	-1.718426
H	-1.467400	-2.644185	-0.915999
C	-2.570069	1.809822	-0.681003
C	-2.337915	2.918156	-1.507433
C	-3.055145	4.107220	-1.338625
C	-4.026094	4.189902	-0.339631
C	-4.288710	3.096552	0.492080
C	-3.560278	1.911449	0.327226
C	-4.741299	0.745581	2.072717
H	-5.741911	0.895891	1.633062
H	-4.686196	-0.260034	2.508404
H	-4.573496	1.493452	2.867002
H	-5.055928	3.173481	1.262320
H	-4.594116	5.113227	-0.202057
H	-2.857484	4.959667	-1.991638
H	-1.596337	2.865170	-2.305584
C	-0.531952	0.444344	-2.274042
C	0.746163	1.235254	-1.972753
C	2.751402	-0.774080	-1.281144
C	2.514878	-1.320972	-2.550139
C	3.276325	-2.391147	-3.032577
C	4.298066	-2.919473	-2.243523
C	4.569554	-2.385000	-0.979640
C	3.799378	-1.318727	-0.496658
C	5.032897	-1.166608	1.562381
H	4.996110	-0.518961	2.448167
H	4.891114	-2.215621	1.875406
H	6.018895	-1.056482	1.079644
H	5.378246	-2.801356	-0.379434
H	4.900484	-3.753863	-2.610831
H	3.072698	-2.801324	-4.023846
H	1.732788	-0.911372	-3.190396
C	2.916063	1.940153	-0.241218
C	4.153000	2.012975	-0.903497
C	5.016266	3.086019	-0.670527
C	4.656099	4.101905	0.221249
C	3.424869	4.041015	0.879060
C	2.561912	2.964456	0.652151
H	1.608144	2.934249	1.180509
H	3.134457	4.830041	1.577150
H	5.334937	4.938718	0.403151
H	5.976685	3.128794	-1.190471
H	4.449820	1.227371	-1.601853
H	1.390252	1.306166	-2.863767
H	0.509633	2.270502	-1.680911
H	-1.099538	0.897804	-3.102200
H	-0.301727	-0.584935	-2.588883
C	-0.653889	1.735402	2.216735
C	0.258432	1.221074	3.076760
H	1.324943	1.445334	2.988109
H	-0.048437	0.642556	3.951391
H	-0.368921	2.413682	1.407834
H	-1.725689	1.594551	2.370576

^{4}9B-18
Geometry with 85 atoms:
Total energy: -3274.489639270

Cr	-0.038706	-0.179892	1.444323
P	-1.587128	-0.189154	-0.653060
P	1.607461	0.598575	-0.545490
O	-2.159158	2.711129	-0.348628
O	2.143445	-2.257047	-0.835462
C	1.502692	-0.334772	2.769943
C	1.607069	-1.735501	2.239897
C	1.307509	-2.890359	3.212236
C	-0.173389	-3.238756	3.412957
C	-1.123434	-2.065392	3.704880
C	-1.531808	-1.256020	2.468294
H	-2.341808	-0.554472	2.726537
H	-1.974996	-1.948850	1.731229
H	-0.688435	-1.415191	4.485814
H	-2.040093	-2.487660	4.159543
H	-0.234440	-3.973130	4.233294
H	-0.546009	-3.766539	2.514784
H	1.829980	-3.795447	2.859302
H	1.764180	-2.634117	4.182703
H	0.890768	-1.882632	1.338739
H	2.568912	-1.888249	1.728560
H	2.384994	0.294016	2.594194
H	1.148327	-0.243361	3.805041
C	-1.963821	-1.843457	-1.368559
C	-2.738007	-1.966527	-2.538113
C	-2.981900	-3.222384	-3.095767
C	-2.458314	-4.373236	-2.493961
C	-1.688567	-4.261282	-1.334271
C	-1.441622	-3.002139	-0.776723
H	-0.837153	-2.921975	0.126552
H	-1.280295	-5.155723	-0.857105
H	-2.653779	-5.355976	-2.930096
H	-3.585558	-3.304692	-4.002898
H	-3.162589	-1.077747	-3.011780
C	-3.229410	0.607544	-0.442175
C	-4.395554	-0.162127	-0.305819
C	-5.633150	0.433200	-0.047559
C	-5.714769	1.819633	0.081464
C	-4.567651	2.611407	-0.029680
C	-3.325024	2.012182	-0.275491
C	-2.168769	4.128813	-0.256076
H	-1.128107	4.453298	-0.390960
H	-2.790326	4.579841	-1.048216
H	-2.527555	4.468669	0.730281
H	-4.648971	3.691811	0.084804
H	-6.676996	2.299362	0.276545
H	-6.526209	-0.187505	0.049611
H	-4.338871	-1.247231	-0.405247
C	-0.757337	0.660923	-2.092142
C	0.722276	0.271773	-2.152175
C	3.255608	-0.177033	-0.808415
C	4.445171	0.560654	-0.900359
C	5.681700	-0.072715	-1.052535
C	5.737520	-1.464577	-1.118701
C	4.567356	-2.225883	-1.044598
C	3.327588	-1.589428	-0.895065
C	2.147150	-3.676787	-0.828487
H	2.565289	-4.084706	-1.764163
H	2.715643	-4.076146	0.029015
H	1.100820	-3.991281	-0.748891
H	4.630856	-3.311252	-1.109485
H	6.697853	-1.972653	-1.235664
H	6.593877	0.523704	-1.120677
H	4.411789	1.649791	-0.853720
C	1.956508	2.404398	-0.535140
C	2.635134	2.935509	0.579271
C	2.879705	4.305345	0.680519
C	2.433526	5.173523	-0.322688
C	1.757211	4.658753	-1.431382
C	1.524392	3.282736	-1.542380
H	1.005708	2.912564	-2.427733
H	1.413603	5.328338	-2.223875
H	2.618055	6.247459	-0.241385
H	3.415637	4.697961	1.548112
H	2.978389	2.268612	1.374284
H	0.836263	-0.809770	-2.321281
H	1.243702	0.781007	-2.977622
H	-0.889012	1.738397	-1.939980
H	-1.272221	0.388001	-3.025742
C	-0.166752	2.287241	2.091896
C	-1.263763	1.752168	2.660219
H	-1.255213	1.395634	3.693796
H	-2.222656	1.722891	2.136264
H	0.766447	2.395507	2.647972
H	-0.200599	2.708340	1.086871

^{4}9C-01
Geometry with 89 atoms:
Total energy: -3202.753274170

Cr	0.034159	-0.991715	1.062167
P	-1.519296	0.396109	-0.366083
C	-2.789175	-0.676127	-1.126696
C	-2.576908	-1.281735	-2.375735
C	-3.503894	-2.197947	-2.879375
C	-4.645956	-2.521725	-2.140849
C	-4.864229	-1.918328	-0.898198
C	-3.941877	-1.000287	-0.391354
H	-4.127643	-0.528936	0.575893
H	-5.758739	-2.160910	-0.319528
H	-5.367153	-3.241748	-2.534692
H	-3.330101	-2.663481	-3.852500
H	-1.687924	-1.050102	-2.965919
C	-2.374977	1.805834	0.441503
C	-1.982885	2.079704	1.766770
C	-2.494279	3.170219	2.467587
C	-3.414297	4.011082	1.836856
C	-3.810952	3.746728	0.526175
C	-3.313803	2.651196	-0.201870
C	-3.828871	2.453778	-1.615024
H	-3.257099	1.679296	-2.139799
C	-5.318203	2.088070	-1.673527
H	-5.945178	2.865001	-1.208617
H	-5.645954	1.972664	-2.718794
H	-5.513960	1.139395	-1.151789
H	-3.664542	3.390744	-2.174728
H	-4.528342	4.413843	0.040611
H	-3.823653	4.875563	2.365401
H	-2.178063	3.359663	3.495858
H	-1.269202	1.420607	2.263560
C	-0.546780	1.162478	-1.769124
C	0.758989	0.427600	-2.095498
P	1.795690	0.226866	-0.556790
C	3.325962	-0.635342	-1.104210
C	3.347024	-1.306321	-2.343111
C	4.454285	-2.057701	-2.737742
C	5.561778	-2.152705	-1.892381
C	5.549442	-1.492740	-0.663724
C	4.448453	-0.729370	-0.242100
C	4.535533	-0.035002	1.103765
C	5.527993	1.134509	1.130981
H	5.241864	1.917324	0.413756
H	6.545575	0.798556	0.876766
H	5.564569	1.589075	2.133842
H	4.835527	-0.776820	1.863274
H	3.545545	0.330955	1.411807
H	6.416891	-1.571801	-0.002319
H	6.433082	-2.742395	-2.187604
H	4.447945	-2.568172	-3.703649
H	2.493842	-1.251207	-3.019925
C	2.255325	1.981416	-0.257413
C	1.631711	2.684894	0.784818
C	1.899322	4.043151	0.982811
C	2.797375	4.706534	0.142253
C	3.424946	4.011267	-0.898329
C	3.155651	2.655795	-1.099999
H	3.655817	2.118784	-1.910326
H	4.129415	4.527498	-1.555164
H	3.009928	5.767198	0.296912
H	1.402028	4.581519	1.793210
H	0.921467	2.181106	1.445129
H	0.553471	-0.570563	-2.508246
H	1.331847	0.989319	-2.849966

H	-1.179765	1.236502	-2.665461
H	-0.334340	2.192789	-1.444176
C	-1.446842	-1.453278	2.404677
C	-1.443408	-2.796939	3.141022
H	-0.435710	-3.039969	3.526682
C	-1.964998	-3.996917	2.341855
C	-1.106343	-4.502755	1.173899
C	-1.098610	-3.648517	-0.107651
C	-0.007618	-2.588841	-0.227133
H	0.996116	-3.037947	-0.096278
H	-0.032488	-2.150822	-1.239196
H	-0.979957	-4.332755	-0.970659
H	-2.092220	-3.190713	-0.246237
H	-0.068107	-4.667561	1.519185
H	-1.485528	-5.503319	0.906810
H	-2.095887	-4.834494	3.049137
H	-2.977855	-3.764877	1.962936
H	-2.075293	-2.706578	4.045960
H	-2.441746	-1.282073	1.960412
H	-1.291804	-0.628266	3.135749
C	1.692839	-1.205655	3.124046
C	2.034595	-2.234290	2.329727
H	1.610572	-3.231767	2.479609
H	2.777469	-2.130839	1.533944
H	0.991168	-1.332468	3.953210
H	2.160464	-0.220690	3.020792

[4]9C-02

Geometry with 89 atoms:

Total energy: -3202.752662830

Cr	0.112267	-0.973204	1.010447
P	-1.533514	0.355311	-0.358026
C	-2.768881	-0.765566	-1.107905
C	-2.562348	-1.338819	-2.372903
C	-3.461690	-2.284679	-2.871932
C	-4.570042	-2.670830	-2.112403
C	-4.781657	-2.101527	-0.852563
C	-3.887194	-1.153677	-0.350511
H	-4.067324	-0.710849	0.631311
H	-5.649614	-2.393974	-0.256737
H	-5.269953	-3.413412	-2.502757
H	-3.292566	-2.724187	-3.857876
H	-1.697410	-1.060674	-2.978320
C	-2.457585	1.691544	0.498035
C	-2.097551	1.924947	1.839651
C	-2.676500	2.953063	2.581380
C	-3.633987	3.770282	1.975797
C	-4.002466	3.542592	0.649956
C	-3.437658	2.509272	-0.118450
C	-3.932528	2.338947	-1.542023
H	-3.315109	1.618044	-2.090113
C	-5.398409	1.893148	-1.627995
H	-6.071228	2.611506	-1.133955
H	-5.713513	1.806992	-2.679965
H	-5.542658	0.912108	-1.151179
H	-3.816453	3.303896	-2.065098
H	-4.752784	4.188654	0.186005
H	-4.096745	4.586093	2.536638
H	-2.383839	3.111946	3.621736
H	-1.357514	1.279657	2.314919
C	-0.638029	1.191101	-1.774559
C	0.700402	0.535043	-2.133180
P	1.777266	0.368998	-0.619100
C	3.348820	-0.376661	-1.213035
C	3.377270	-1.048757	-2.449194
C	4.529557	-1.703140	-2.887720
C	5.672330	-1.691290	-2.088213
C	5.653924	-1.029351	-0.858417
C	4.509647	-0.363928	-0.392174
C	4.537785	0.371112	0.936314
C	5.497798	-0.172162	1.994944
H	5.353036	0.362356	2.946756
H	6.551968	-0.036535	1.708878
H	5.335199	-1.245742	2.181809
H	3.519306	0.388540	1.353839
H	4.769511	1.433367	0.743055
H	6.557880	-1.032244	-0.247527
H	6.581831	-2.199399	-2.417975
H	4.529017	-2.219213	-3.850627
H	2.494249	-1.074660	-3.088582
C	2.126353	2.141321	-0.280335
C	1.382630	2.795758	0.713966
C	1.563241	4.161327	0.953454
C	2.499712	4.881209	0.206310
C	3.249027	4.234528	-0.783962
C	3.062498	2.872363	-1.031005
H	3.653597	2.375318	-1.804868
H	3.982856	4.795233	-1.368287
H	2.647860	5.947335	0.394865
H	0.971000	4.659493	1.724901
H	0.644323	2.244198	1.301117
H	0.541420	-0.467804	-2.554717
H	1.226775	1.135324	-2.891706
H	-1.291699	1.229303	-2.658101
H	-0.483971	2.231242	-1.448516
C	-1.293097	-1.523121	2.397569
C	-1.226636	-2.894167	3.078920
H	-0.201305	-3.119898	3.426440
C	-1.734241	-4.081428	2.251644
C	-0.879990	-4.539891	1.060979
C	-0.915780	-3.664945	-0.204619
C	0.113656	-2.544364	-0.305470
H	1.141719	-2.939813	-0.184697
H	0.060408	-2.090392	-1.309678
H	-0.756923	-4.327546	-1.078059
H	-1.933084	-3.262038	-0.338983
H	0.167533	-4.682880	1.387793
H	-1.235700	-5.545302	0.779675
H	-1.837750	-4.940449	2.937274
H	-2.756846	-3.861382	1.892465
H	-1.833536	-2.857044	4.004598
H	-2.313490	-1.357084	2.011934
H	-1.119021	-0.726016	3.154836
C	1.851734	-1.171081	3.062932
C	2.249602	-2.149521	2.232708
H	1.907426	-3.180386	2.363835
H	2.965650	-1.970164	1.425565
H	1.180919	-1.372078	3.902664
H	2.237558	-0.149085	2.975640

[4]9C-03

Geometry with 89 atoms:

Total energy: -3202.754187780

Cr	0.179948	-0.983538	1.265298
P	-1.571672	0.241306	-0.291741
C	-2.839374	-0.955731	-0.858924
C	-2.587567	-1.812867	-1.944087
C	-3.507371	-2.807228	-2.287471
C	-4.684983	-2.961600	-1.549607
C	-4.941900	-2.112445	-0.469025
C	-4.026035	-1.115500	-0.122782
H	-4.243684	-0.454759	0.719175
H	-5.862363	-2.223788	0.109111
H	-5.401687	-3.741348	-1.817573
H	-3.301301	-3.464353	-3.135918
H	-1.672103	-1.716852	-2.532362
C	-2.492779	1.699376	0.347686
C	-2.208904	2.058655	1.679770
C	-2.785617	3.180561	2.272968
C	-3.662947	3.967915	1.523882
C	-3.965538	3.610358	0.210030
C	-3.408586	2.475685	-0.406286
C	-3.851505	2.151947	-1.820298
H	-3.264113	1.325439	-2.235722
C	-5.339572	1.789133	-1.922067
H	-5.569174	0.893439	-1.325039
H	-5.984832	2.607503	-1.566320
H	-5.613221	1.577595	-2.967912
H	-3.647137	3.028441	-2.459561
H	-4.660095	4.229775	-0.363962
H	-4.117975	4.858673	1.964169
H	-2.551239	3.436093	3.308971
H	-1.527793	1.439978	2.263444
C	-0.692437	0.812179	-1.843748
C	0.647492	0.103118	-2.074282
P	1.732406	0.198272	-0.559820
C	3.308673	-0.612069	-1.047992
C	3.419480	-1.290728	-2.277403
C	4.582335	-1.984315	-2.615613
C	5.656077	-2.009845	-1.723198
C	5.555131	-1.340687	-0.503425
C	4.396195	-0.636959	-0.139153
C	4.375218	0.070366	1.201391
C	5.324216	1.272404	1.286737
H	6.366858	0.973332	1.096047
H	5.283500	1.727780	2.289084
H	5.054879	2.045031	0.551887
H	4.649437	-0.658930	1.983235
H	3.354827	0.404170	1.438661
H	6.396186	-1.366352	0.195111
H	6.570374	-2.552543	-1.975433
H	4.646702	-2.501462	-3.575886
H	2.597921	-1.284130	-2.994187
C	2.086078	2.002195	-0.488229
C	1.269754	2.827006	0.304976
C	1.472123	4.209859	0.332877
C	2.498220	4.781129	-0.425157
C	3.314883	3.967149	-1.218058
C	3.110604	2.585292	-1.253708
H	3.756653	1.959332	-1.873791
H	4.117242	4.410660	-1.812839
H	2.662692	5.861100	-0.399477
H	0.825461	4.838238	0.950205
H	0.459969	2.395911	0.896298
H	0.491799	-0.964461	-2.296901
H	1.166015	0.552648	-2.935909
H	-1.343345	0.675688	-2.719191
H	-0.539040	1.895880	-1.725287
C	-1.363425	-1.826615	2.393589
C	-1.521955	-3.351521	2.442816
H	-0.677626	-3.817665	2.982019
C	-1.695334	-4.031346	1.073944
C	-0.411193	-4.258086	0.263727
C	0.495837	-3.026326	0.090592
C	1.384477	-2.645668	1.237103
H	1.308452	-3.288023	2.121014
H	2.428539	-2.445614	0.967676
H	1.065815	-3.071670	-0.852278
H	-0.239699	-2.164001	-0.160454
H	0.193785	-5.053396	0.730490
H	-0.693218	-4.629148	-0.735448
H	-2.174490	-5.014602	1.213596
H	-2.402038	-3.436012	0.471036
H	-2.416732	-3.589401	3.049136
H	-2.304666	-1.386336	2.020603
H	-1.228052	-1.430498	3.416680
C	0.944601	0.429254	3.101006
C	1.523762	-0.762818	3.380519
H	1.019096	-1.513740	3.992890
H	2.556964	-0.977348	3.102861
H	-0.033654	0.685733	3.517016
H	1.497549	1.227876	2.598705

[4]9C-04

Geometry with 89 atoms:

Total energy: -3202.749827950

Cr	-0.197296	-1.295828	1.122632
P	-1.539298	0.268893	-0.331134
C	-3.208210	-0.232821	-0.890167
C	-3.397267	-0.931921	-2.094284
C	-4.666910	-1.396933	-2.446522
C	-5.758007	-1.171143	-1.602407
C	-5.577252	-0.471212	-0.405363
C	-4.310707	-0.004434	-0.047798
H	-4.183701	0.543238	0.888391
H	-6.426943	-0.286474	0.256174
H	-6.749321	-1.538151	-1.878673
H	-4.802121	-1.939179	-3.385408
H	-2.559572	-1.127374	-2.767036
C	-1.786937	1.816875	0.635268
C	-1.438189	1.761752	1.999676
C	-1.581529	2.866968	2.836180
C	-2.092931	4.055386	2.308653
C	-2.451087	4.118235	0.962363
C	-2.310856	3.017680	0.098306
C	-2.708962	3.200807	-1.352004
H	-3.726251	3.626257	-1.378981
C	-1.761333	4.131749	-2.122440
H	-1.752211	5.142673	-1.685897
H	-0.722910	3.764216	-2.107228
H	-2.075777	4.223447	-3.174117
H	-2.784940	2.231917	-1.862780
H	-2.860357	5.049496	0.561198

H	-2.221052	4.931974	2.948430
H	-1.303360	2.797764	3.890236
H	-1.041401	0.836904	2.428415
C	-0.554505	0.708157	-1.859911
C	0.685058	-0.177596	-2.025750
P	1.700399	-0.135943	-0.461960
C	3.235445	-1.070434	-0.862045
C	3.299921	-1.870935	-2.019558
C	4.426107	-2.647072	-2.296764
C	5.507138	-2.637458	-1.412847
C	5.448985	-1.852963	-0.260753
C	4.327541	-1.064057	0.041614
C	4.358235	-0.221679	1.301270
C	5.263926	1.011676	1.189040
H	6.304569	0.718651	0.978183
H	5.258209	1.586658	2.128753
H	4.931259	1.677763	0.379579
H	4.703551	-0.849850	2.139720
H	3.340956	0.103744	1.564714
H	6.294572	-1.850669	0.433054
H	6.393116	-3.243117	-1.618294
H	4.454647	-3.258031	-3.202086
H	2.467162	-1.901497	-2.722935
C	2.185784	1.638392	-0.426619
C	1.755828	2.454990	0.628990
C	2.050770	3.822010	0.633870
C	2.784939	4.380754	-0.415397
C	3.227759	3.570139	-1.468411
C	2.930442	2.205869	-1.475548
H	3.289037	1.577682	-2.295202
H	3.809569	4.003557	-2.285598
H	3.016947	5.448610	-0.413599
H	1.701046	4.448058	1.458226
H	1.177292	2.033139	1.452428
H	0.398345	-1.222419	-2.218414
H	1.285637	0.170142	-2.880682
H	-1.199864	0.648677	-2.747727
H	-0.254186	1.759129	-1.753216
C	-1.862804	-1.840106	2.211357
C	-2.426548	-3.262541	2.102007
H	-1.655891	-4.008353	2.371308
C	-3.044142	-3.637295	0.738976
C	-2.117433	-4.306344	-0.286280
C	-0.979399	-3.471178	-0.885187
C	0.109076	-3.027676	0.087387
H	0.252527	-3.766813	0.895735
H	1.081514	-2.901595	-0.418792
H	-0.512043	-4.074290	-1.687906
H	-1.411451	-2.600192	-1.409891
H	-1.679248	-5.213769	0.170085
H	-2.744540	-4.664336	-1.121669
H	-3.872703	-4.342571	0.920864
H	-3.511895	-2.744587	0.289814
H	-3.213177	-3.375671	2.872392
H	-2.675060	-1.116569	2.017152
H	-1.532673	-1.654111	3.254004
C	1.316999	-1.133092	3.344075
C	1.706171	-2.280882	2.764030
H	1.283290	-3.241248	3.074198
H	2.486954	-2.310018	1.997946
H	0.573514	-1.124813	4.147279
H	1.776814	-0.172365	3.089074

^{49}C-05

Geometry with 89 atoms:

Total energy: -3202.754868930

Cr	0.126699	-1.005116	1.252706
P	-1.616297	0.215435	-0.296553
C	-2.791426	-1.023676	-0.971598
C	-2.425910	-1.846164	-2.051299
C	-3.275392	-2.869554	-2.479609
C	-4.495921	-3.087234	-1.832985
C	-4.867477	-2.270110	-0.761093
C	-4.021974	-1.244807	-0.330004
H	-4.326835	-0.610379	0.504942
H	-5.822540	-2.430184	-0.254909
H	-5.157676	-3.889899	-2.166741
H	-2.981207	-3.499230	-3.322874
H	-1.476556	-1.698147	-2.569103
C	-2.655972	1.559432	0.404123
C	-2.481357	1.802752	1.780262
C	-3.201824	2.795367	2.443016
C	-4.124899	3.558600	1.724661
C	-4.318782	3.313489	0.364862
C	-3.604023	2.319686	-0.326270
C	-3.886348	2.145068	-1.804546
H	-4.979931	2.125128	-1.945452
C	-3.297312	3.268415	-2.669089
H	-3.713673	4.248035	-2.385853
H	-2.203780	3.334550	-2.562709
H	-3.526099	3.101556	-3.733795
H	-3.529100	1.168800	-2.157237
H	-5.055298	3.905956	-0.185462
H	-4.703557	4.339089	2.224980
H	-3.049804	2.963595	3.511678
H	-1.778945	1.187861	2.342712
C	-0.729881	0.926538	-1.781938
C	0.622833	0.257368	-2.050071
P	1.685633	0.240302	-0.517016
C	3.264077	-0.543724	-1.042487
C	3.392853	-1.115067	-2.324106
C	4.554157	-1.792706	-2.697752
C	5.608427	-1.910498	-1.789565
C	5.491963	-1.343510	-0.520559
C	4.335118	-0.655677	-0.120454
C	4.301237	-0.053961	1.270638
C	5.265606	1.123504	1.462992
H	6.307133	0.823799	1.267288
H	5.213826	1.501673	2.496479
H	5.021049	1.954815	0.785394
H	4.551264	-0.845322	1.998229
H	3.281876	0.275444	1.516664
H	6.319137	-1.438162	0.188571
H	6.520434	-2.443730	-2.068814
H	4.632679	-2.225235	-3.697989
H	2.587774	-1.035128	-3.055195
C	2.043148	2.036034	-0.329742
C	1.183499	2.827538	0.452966
C	1.388660	4.206410	0.557191
C	2.457690	4.807217	-0.114000
C	3.315540	4.027180	-0.896906
C	3.109756	2.649495	-1.008703
H	3.786036	2.049608	-1.622272
H	4.150846	4.493726	-1.424981
H	2.622972	5.883934	-0.027928
H	0.711002	4.809518	1.166401
H	0.340347	2.373875	0.978639
H	0.490577	-0.788803	-2.366482
H	1.149518	0.785135	-2.860719
H	-1.369999	0.863569	-2.673374
H	-0.584275	1.994952	-1.563511
C	-1.447595	-1.877238	2.314526
C	-1.554640	-3.406740	2.374775
H	-0.706912	-3.841447	2.934578
C	-1.680309	-4.100248	1.006883
C	-0.375216	-4.292087	0.220843
C	0.499914	-3.034416	0.071807
C	1.361021	-2.645820	1.235283
H	1.282191	-3.296607	2.112602
H	2.404541	-2.419470	0.986132
H	1.082221	-3.051190	-0.864296
H	-0.260663	-2.192784	-0.173560
H	0.241505	-5.072734	0.696796
H	-0.628271	-4.666409	-0.784651
H	-2.133005	-5.096356	1.143259
H	-2.392195	-3.528484	0.387017
H	-2.453654	-3.669111	2.964536
H	-2.387404	-1.479036	1.894387
H	-1.373105	-1.463556	3.337331
C	0.861432	0.393898	3.106075
C	1.383603	-0.815590	3.421314
H	0.823994	-1.547255	4.008862
H	2.423308	-1.064863	3.202889
H	-0.126136	0.692324	3.468383
H	1.469918	1.168328	2.631108

^{49}C-06

Geometry with 89 atoms:

Total energy: -3202.751077030

Cr	0.206214	-0.902689	1.202485
P	-1.287651	0.260136	-0.500735
C	-2.524784	-0.925198	-1.138207
C	-2.243890	-1.751187	-2.238648
C	-3.159990	-2.728505	-2.635409
C	-4.357820	-2.896185	-1.934001
C	-4.639564	-2.080088	-0.833915
C	-3.728728	-1.098937	-0.435037
H	-3.959227	-0.465947	0.424868
H	-5.574106	-2.206031	-0.282172
H	-5.070909	-3.663447	-2.244382
H	-2.933075	-3.365046	-3.494007
H	-1.306438	-1.651634	-2.790364
C	-2.207987	1.756003	0.044629
C	-1.900942	2.240231	1.330011
C	-2.480474	3.406771	1.825557
C	-3.381763	4.111534	1.025824
C	-3.688161	3.642779	-0.251740
C	-3.119857	2.468892	-0.776227
C	-3.522466	2.062093	-2.182265
H	-2.922541	1.216310	-2.537858
C	-5.007069	1.697975	-2.316767
H	-5.659797	2.538494	-2.033886
H	-5.243829	1.426056	-3.357612
H	-5.263993	0.840563	-1.676873
H	-3.295417	2.903705	-2.859802
H	-4.387143	4.208885	-0.873399
H	-3.844591	5.030864	1.393204
H	-2.224282	3.762026	2.826173
H	-1.191188	1.699763	1.954482
C	-0.297926	0.850185	-1.983758
C	1.142052	0.330025	-2.044488
P	1.958600	0.338582	-0.370231
C	3.761962	0.077086	-0.659084
C	4.667336	1.119826	-0.377977
C	6.043071	0.932916	-0.512467
C	6.536161	-0.306788	-0.926411
C	5.646794	-1.344836	-1.202485
C	4.257254	-1.182980	-1.075457
C	3.363724	-2.353749	-1.424694
C	3.263170	-2.607606	-2.935388
H	2.892228	-1.718921	-3.470503
H	2.582155	-3.447336	-3.147814
H	4.247948	-2.855646	-3.361362
H	2.357647	-2.207809	-1.008240
H	3.756919	-3.261582	-0.936708
H	6.034821	-2.316321	-1.521781
H	7.612193	-0.466906	-1.029479
H	6.726277	1.755982	-0.289952
H	4.298768	2.091600	-0.047051
C	1.817526	2.081751	0.198754
C	1.692560	2.322776	1.579146
C	1.545616	3.623921	2.066643
C	1.514706	4.701719	1.177790
C	1.647896	4.475619	-0.196465
C	1.805037	3.176014	-0.683742
H	1.925836	3.020563	-1.758312
H	1.632966	5.316918	-0.893606
H	1.389823	5.719411	1.555124
H	1.449668	3.794785	3.141509
H	1.719507	1.490946	2.289296
H	1.163829	-0.715700	-2.383867
H	1.734516	0.911277	-2.768173
H	-0.835041	0.593524	-2.907859
H	-0.307807	1.945956	-1.906971
C	-1.285333	-0.982384	2.620754
C	-1.615311	-2.168169	3.530250
H	-0.726573	-2.503079	4.092663
C	-2.249509	-3.385125	2.846507
C	-1.364007	-4.224233	1.910880
C	-1.128257	-3.674924	0.493337
C	0.046183	-2.724080	0.296431
H	0.989172	-3.205537	0.620357
H	0.157817	-2.481771	-0.777372
H	-0.960874	-4.538961	-0.179487
H	-2.059665	-3.213881	0.131196
H	-0.394511	-4.435314	2.401395
H	-1.852910	-5.206975	1.802688
H	-2.618457	-4.052847	3.644430
H	-3.148617	-3.062465	2.289182
H	-2.325595	-1.823748	4.307267
H	-2.211879	-0.662860	2.109999
H	-0.966789	-0.115379	3.243212
C	2.625433	-1.411459	2.275445

C	1.671637	-1.804527	3.140165
H	1.363994	-1.176453	3.981691
H	1.234561	-2.804444	3.088771
H	3.140588	-0.451427	2.377065
H	2.994978	-2.069317	1.484238

^{4}9C-07
Geometry with 89 atoms:
Total energy: -3202.749829700

Cr	-0.051457	-1.178416	1.157261
P	-1.525590	0.214964	-0.358481
C	-3.174805	-0.401348	-0.851908
C	-3.362755	-1.154517	-2.022798
C	-4.610801	-1.715994	-2.305703
C	-5.680253	-1.535873	-1.423558
C	-5.500630	-0.784399	-0.258084
C	-4.256212	-0.219773	0.028837
H	-4.130764	0.369015	0.939777
H	-6.333234	-0.635237	0.433476
H	-6.653902	-1.979195	-1.645252
H	-4.745984	-2.298976	-3.219763
H	-2.539853	-1.319215	-2.721898
C	-1.823721	1.794859	0.538528
C	-1.378806	1.841417	1.874352
C	-1.466733	3.006090	2.634694
C	-2.005794	4.155774	2.052149
C	-2.471251	4.114264	0.737911
C	-2.410091	2.945647	-0.041851
C	-3.009921	2.989171	-1.433636
H	-2.768385	2.081025	-1.998969
C	-4.536045	3.159834	-1.421986
H	-4.837689	4.086559	-0.909161
H	-4.926257	3.203239	-2.451061
H	-5.023223	2.315866	-0.910420
H	-2.554183	3.828862	-1.986147
H	-2.902634	5.016310	0.295594
H	-2.071211	5.084488	2.624334
H	-1.112607	3.016458	3.667963
H	-0.945606	0.951016	2.340789
C	-0.582017	0.655386	-1.915836
C	0.714300	-0.150522	-2.056116
P	1.746259	-0.017689	-0.509568
C	3.287802	-0.948537	-0.899707
C	3.371309	-1.743883	-2.059465
C	4.504327	-2.513999	-2.325337
C	5.573702	-2.503470	-1.427564
C	5.498645	-1.720690	-0.275294
C	4.370542	-0.936444	0.014819
C	4.388246	-0.087752	1.270317
C	5.284299	1.152651	1.155077
H	5.275748	1.728603	2.094174
H	4.945799	1.815594	0.345518
H	6.326814	0.867078	0.943143
H	4.736889	-0.708131	2.113202
H	3.367169	0.229695	1.528944
H	6.336541	-1.715332	0.427745
H	6.464177	-3.105769	-1.623249
H	4.546736	-3.121328	-3.232599
H	2.550183	-1.774515	-2.776078
C	2.231690	1.755617	-0.549215
C	1.783241	2.623610	0.456884
C	2.109938	3.982849	0.417361
C	2.892404	4.482435	-0.626854
C	3.348967	3.621063	-1.632472
C	3.021339	2.264441	-1.595481
H	3.394724	1.595309	-2.375166
H	3.966475	4.008322	-2.446682
H	3.151097	5.543702	-0.658290
H	1.748024	4.649303	1.203993
H	1.165344	2.247737	1.274070
H	0.491321	-1.216404	-2.215022
H	1.287346	0.207141	-2.925947
H	-1.225167	0.504664	-2.794820
H	-0.362072	1.731910	-1.860610
C	-1.655695	-1.822060	2.285568
C	-2.139078	-3.276587	2.218378
H	-1.324047	-3.969567	2.497842
C	-2.749418	-3.725223	0.875439
C	-1.792117	-4.348444	-0.150382
C	-0.714186	-3.448817	-0.765894
C	0.358567	-2.937678	0.192657
H	0.531481	-3.651628	1.016236
H	1.324088	-2.789805	-0.319293
H	-0.221339	-4.022943	-1.574467
H	-1.206610	-2.607502	-1.285977
H	-1.293978	-5.220975	0.312283
H	-2.402848	-4.754083	-0.976069
H	-3.522909	-4.483046	1.086361
H	-3.285444	-2.878103	0.414994
H	-2.909149	-3.413201	3.001573
H	-2.512217	-1.151812	2.086575
H	-1.332242	-1.596348	3.321162
C	1.741379	-2.029648	2.894646
C	1.366547	-0.814073	3.330470
H	1.893828	0.092849	3.017315
H	0.576976	-0.693599	4.078299
H	2.569473	-2.158782	2.190783
H	1.256763	-2.938642	3.263593

^{4}9C-08
Geometry with 89 atoms:
Total energy: -3202.749630560

Cr	-0.205917	-1.377277	1.061286
P	-1.492740	0.310297	-0.338012
C	-3.174920	-0.107575	-0.935046
C	-3.373979	-0.742058	-2.173453
C	-4.655625	-1.136091	-2.566308
C	-5.750654	-0.902917	-1.729323
C	-5.560703	-0.266445	-0.498853
C	-4.281775	0.129571	-0.100941
H	-4.150005	0.633689	0.858703
H	-6.413169	-0.074316	0.156973
H	-6.751895	-1.213045	-2.037813
H	-4.796805	-1.627890	-3.531777
H	-2.535165	-0.939138	-2.844296
C	-1.703480	1.830760	0.680985
C	-1.357902	1.720282	2.042657
C	-1.487923	2.794561	2.920461
C	-1.979651	4.009690	2.437188
C	-2.329881	4.129355	1.092811
C	-2.204289	3.060299	0.187924
C	-2.591759	3.309855	-1.255452
H	-3.604208	3.747360	-1.270365
C	-1.627786	4.262346	-1.977851
H	-1.932586	4.403629	-3.026878
H	-1.610208	5.253064	-1.497424
H	-0.593843	3.882378	-1.970128
H	-2.674800	2.365830	-1.809346
H	-2.721323	5.081957	0.725465
H	-2.097573	4.862932	3.109689
H	-1.214396	2.681065	3.971885
H	-0.975903	0.774218	2.435098
C	-0.492964	0.775265	-1.851517
C	0.730101	-0.128962	-2.036413
P	1.721183	-0.155505	-0.457428
C	3.268669	-1.062979	-0.863593
C	3.324253	-1.869664	-2.017655
C	4.453582	-2.636152	-2.307576
C	5.547089	-2.610198	-1.439475
C	5.497869	-1.818889	-0.291798
C	4.373869	-1.038478	0.024459
C	4.424735	-0.190684	1.281042
C	5.330496	1.040603	1.149891
H	6.366307	0.747566	0.916706
H	5.344920	1.615058	2.089863
H	4.980902	1.708183	0.348740
H	4.785452	-0.819364	2.112750
H	3.415789	0.138133	1.566912
H	6.354073	-1.804109	0.388722
H	6.436371	-3.207871	-1.653888
H	4.475291	-3.251571	-3.210022
H	2.481386	-1.909725	-2.708480
C	2.188012	1.621921	-0.338992
C	1.799094	2.373060	0.778836
C	2.079213	3.741249	0.847184
C	2.756695	4.367240	-0.202246
C	3.160553	3.621808	-1.317164
C	2.879157	2.255703	-1.386443
H	3.209045	1.679386	-2.254974
H	3.700145	4.107275	-2.134036
H	2.975753	5.436650	-0.152030
H	1.762266	4.315659	1.720855
H	1.269101	1.894944	1.603680
H	0.425488	-1.160151	-2.269619
H	1.350309	0.234677	-2.870123
H	-1.135390	0.751320	-2.742768
H	-0.172283	1.816755	-1.717223
C	-1.915667	-1.791689	2.152203
C	-2.520183	-3.199041	2.131469
H	-1.767005	-3.960837	2.404825
C	-3.198176	-3.606222	0.808549
C	-2.325968	-4.297111	-0.248487
C	-1.259239	-3.459467	-0.965134
C	-0.057842	-3.034450	-0.129516
H	0.243349	-3.836412	0.567227
H	0.818692	-2.828403	-0.769255
H	-0.892412	-4.057371	-1.822406
H	-1.744401	-2.580036	-1.420318
H	-1.836353	-5.177910	0.208466
H	-3.002520	-4.700999	-1.021834
H	-4.016817	-4.305704	1.048696
H	-3.685881	-2.722034	0.360966
H	-3.284332	-3.253787	2.930402
H	-2.699120	-1.070648	1.861225
H	-1.626657	-1.514143	3.186316
C	1.790219	-1.991737	2.537848
C	0.855168	-2.781123	3.098089
H	0.284801	-2.464609	3.975387
H	0.668845	-3.796775	2.739323
H	2.027869	-1.009348	2.958719
H	2.423841	-2.342587	1.717982

^{4}9C-09
Geometry with 89 atoms:
Total energy: -3202.750957460

Cr	0.137783	-1.020644	1.166614
P	-1.383961	0.233878	-0.416506
C	-2.557273	-0.927910	-1.205132
C	-2.221585	-1.615390	-2.382865
C	-3.089590	-2.577021	-2.906239
C	-4.295012	-2.863343	-2.258470
C	-4.634380	-2.179632	-1.086405
C	-3.770791	-1.217285	-0.558777
H	-4.048691	-0.685300	0.353874
H	-5.577302	-2.395673	-0.578365
H	-4.971288	-3.617247	-2.668318
H	-2.820437	-3.106691	-3.823269
H	-1.280453	-1.413898	-2.899850
C	-2.392931	1.610410	0.266856
C	-2.201271	1.913107	1.628304
C	-2.913749	2.934627	2.253866
C	-3.843567	3.668199	1.514356
C	-4.036762	3.379951	0.163243
C	-3.322837	2.363679	-0.494758
C	-3.571440	2.176523	-1.978204
H	-4.660751	2.128398	-2.144410
C	-2.988296	3.312411	-2.830807
H	-3.193507	3.140732	-3.899571
H	-3.426570	4.284927	-2.556838
H	-1.897800	3.396732	-2.703324
H	-3.179836	1.212389	-2.325031
H	-4.766067	3.960301	-0.408966
H	-4.421020	4.465253	1.989292
H	-2.748280	3.148297	3.312285
H	-1.486356	1.337165	2.214620
C	-0.383768	0.996327	-1.806501
C	1.045789	0.453479	-1.932960
P	1.876039	0.409722	-0.260100
C	3.687875	0.142364	-0.511524
C	4.589510	1.092294	0.011730
C	5.968320	0.896905	-0.063087
C	6.471978	-0.259938	-0.661899
C	5.588065	-1.209082	-1.173623
C	4.194827	-1.039758	-1.107114
C	3.319085	-2.117495	-1.709058
C	3.286419	-2.082882	-3.243403
H	4.290338	-2.251804	-3.663570
H	2.936598	-1.108277	-3.618903
H	2.618619	-2.864577	-3.640024
H	2.297555	-2.048320	-1.314352
H	3.692979	-3.102605	-1.383190
H	5.982714	-2.117789	-1.637180
H	7.550153	-0.425953	-0.725249

H	6.645452	1.649703	0.347497
H	4.215019	2.001047	0.484416
C	1.740191	2.165908	0.276898
C	1.379592	2.447596	1.604000
C	1.228001	3.767182	2.041380
C	1.433872	4.822624	1.150865
C	1.801463	4.555701	-0.173690
C	1.957360	3.238368	-0.608118
H	2.257158	3.050087	-1.641648
H	1.970049	5.379719	-0.871239
H	1.310567	5.854974	1.486910
H	0.943376	3.967601	3.076883
H	1.216817	1.632505	2.313808
H	1.043024	-0.573839	-2.321635
H	1.625789	1.064705	-2.641037
H	-0.928708	0.882326	-2.754806
H	-0.359821	2.070977	-1.578824
C	-1.352225	-1.426376	2.505453
C	-1.338865	-2.734438	3.302238
H	-0.322558	-2.967343	3.672428
C	-1.891778	-3.964094	2.572053
C	-1.053415	-4.555179	1.429591
C	-0.998136	-3.755502	0.115624
C	0.100109	-2.704307	0.000604
H	1.087121	-3.156757	0.208884
H	0.138255	-2.300208	-1.026605
H	-0.849026	-4.475529	-0.712822
H	-1.985327	-3.305628	-0.075714
H	-0.025842	-4.756850	1.787939
H	-1.479689	-5.546023	1.199000
H	-2.038203	-4.759705	3.323362
H	-2.901114	-3.728199	2.185902
H	-1.945591	-2.598038	4.218490
H	-2.347977	-1.273245	2.053798
H	-1.189487	-0.568468	3.196835
C	1.883364	-1.132238	3.194868
C	2.194730	-2.225159	2.479276
H	1.735592	-3.196374	2.684228
H	2.958157	-2.191240	1.695316
H	1.168005	-1.171031	4.021935
H	2.403125	-0.183542	3.025943

^{4}9C-10
Geometry with 89 atoms:
Total energy: -3202.752220480

Cr	0.079887	-0.943393	1.051176
P	-1.745563	-0.052667	-0.368160
C	-2.724974	-1.436414	-1.053878
C	-2.386885	-2.045277	-2.273177
C	-3.121269	-3.139235	-2.738648
C	-4.192068	-3.637486	-1.990640
C	-4.528038	-3.038261	-0.772241
C	-3.798226	-1.944442	-0.301747
H	-4.073560	-1.480337	0.648069
H	-5.365428	-3.421843	-0.184432
H	-4.765481	-4.492075	-2.357579
H	-2.854837	-3.603108	-3.691446
H	-1.553950	-1.673564	-2.872264
C	-2.956717	1.126512	0.359290
C	-2.779661	1.433729	1.721973
C	-3.620642	2.326245	2.385245
C	-4.671397	2.919392	1.682840
C	-4.864209	2.610869	0.336127
C	-4.026030	1.721059	-0.358437
C	-4.317692	1.488392	-1.827288
H	-5.397531	1.292239	-1.935460
C	-3.941518	2.686008	-2.712244
H	-4.175356	2.478371	-3.768595
H	-4.496429	3.590422	-2.416891
H	-2.868452	2.922784	-2.641648
H	-3.819757	0.579940	-2.189659
H	-5.697624	3.070286	-0.202662
H	-5.348189	3.615417	2.184561
H	-3.461569	2.544732	3.443836
H	-1.978215	0.951597	2.277717
C	-0.973979	0.854329	-1.805789
C	0.445227	0.404262	-2.166355
P	1.579672	0.374896	-0.684285
C	3.167479	-0.292871	-1.336267
C	3.340026	-0.505069	-2.718542
C	4.523499	-1.042870	-3.224797
C	5.559687	-1.378949	-2.350921
C	5.399852	-1.171508	-0.981405
C	4.218480	-0.631983	-0.447411
C	4.142454	-0.420059	1.048629
C	4.910780	0.813216	1.540848
H	5.976966	0.747501	1.272101
H	4.846189	0.901802	2.637065
H	4.512031	1.738751	1.099293
H	4.536565	-1.317900	1.553068
H	3.092228	-0.337282	1.357936
H	6.209891	-1.439324	-0.297152
H	6.489468	-1.805521	-2.735016
H	4.632616	-1.198582	-4.300680
H	2.551422	-0.248128	-3.425593
C	1.872723	2.167361	-0.389271
C	0.918440	2.886161	0.354518
C	1.081610	4.254303	0.585830
C	2.207520	4.917838	0.087808
C	3.161313	4.211015	-0.651448
C	2.995246	2.844245	-0.894754
H	3.747264	2.303121	-1.473228
H	4.042263	4.725957	-1.042566
H	2.342476	5.985473	0.277428
H	0.330658	4.799682	1.162818
H	0.040508	2.379869	0.761912
H	0.446168	-0.612052	-2.587260
H	0.855881	1.082269	-2.930207
H	-1.630446	0.784069	-2.684955
H	-0.966687	1.910755	-1.498274
C	-1.216964	-1.853064	2.381295
C	-0.472510	-2.684603	3.436452
H	0.078249	-2.018697	4.129269
C	0.520291	-3.698135	2.850549
C	1.657778	-3.044488	2.031008
C	1.574761	-3.219027	0.498188
C	0.331301	-2.590918	-0.131503
H	0.461065	-2.404402	-1.208362
H	-0.572027	-3.204226	0.001225
H	2.482682	-2.784739	0.047997
H	1.616897	-4.302747	0.278981
H	1.723848	-1.962411	2.304982
H	2.638669	-3.421873	2.362210
H	0.953605	-4.290431	3.672467
H	-0.023266	-4.416109	2.211883
H	-1.199299	-3.224382	4.073719
H	-1.889336	-2.501412	1.792922
H	-1.855225	-1.097803	2.873393
C	1.591308	0.813296	3.181762
C	0.322369	1.093979	3.500175
H	-0.164931	2.001031	3.131967
H	-0.259548	0.456976	4.172367
H	2.177808	1.476273	2.540209
H	2.106622	-0.057685	3.598340

^{4}9C-11
Geometry with 89 atoms:
Total energy: -3202.748796720

Cr	-0.075582	-1.242465	1.156942
P	-1.496069	0.234586	-0.330978
C	-3.145283	-0.343786	-0.875575
C	-3.320844	-1.051307	-2.076764
C	-4.575398	-1.564898	-2.415450
C	-5.665188	-1.382835	-1.559041
C	-5.498754	-0.676337	-0.363987
C	-4.247671	-0.158285	-0.022233
H	-4.134707	0.401888	0.908091
H	-6.347472	-0.523700	0.306869
H	-6.644394	-1.788159	-1.824603
H	-4.699813	-2.111109	-3.353489
H	-2.484033	-1.214366	-2.759202
C	-1.799096	1.797909	0.594893
C	-1.387406	1.812512	1.941970
C	-1.490758	2.959252	2.726960
C	-2.008695	4.125058	2.157714
C	-2.438607	4.116522	0.830901
C	-2.364987	2.965370	0.026535
C	-2.929845	3.046126	-1.378448
H	-2.692144	2.144140	-1.954502
C	-4.452133	3.245611	-1.402390
H	-4.751046	4.167600	-0.879769
H	-4.814436	3.315725	-2.440153
H	-4.967869	2.401415	-0.920149
H	-2.444296	3.886610	-1.903803
H	-2.852544	5.031481	0.398434
H	-2.084777	5.040627	2.749421
H	-1.164206	2.943184	3.769202
H	-0.971191	0.908480	2.396488
C	-0.532963	0.699416	-1.868862
C	0.745519	-0.130713	-2.018136
P	1.769759	-0.028704	-0.462590
C	3.327806	-0.924777	-0.874541
C	3.354138	-1.805567	-1.975502
C	4.486320	-2.566855	-2.266289
C	5.615845	-2.462580	-1.452133
C	5.597956	-1.597514	-0.358592
C	4.471591	-0.819153	-0.043210
C	4.565721	0.110957	1.151367
C	5.469755	1.325984	0.907042
H	6.495285	1.014021	0.653938
H	5.521606	1.959562	1.806800
H	5.091141	1.942602	0.078699
H	4.953252	-0.462700	2.010405
H	3.568873	0.464363	1.447911
H	6.482554	-1.520909	0.279961
H	6.508034	-3.055930	-1.666511
H	4.481486	-3.239967	-3.126888
H	2.485198	-1.912157	-2.625011
C	2.198789	1.759944	-0.457903
C	1.782040	2.573039	0.605893
C	2.052944	3.944818	0.597307
C	2.747479	4.511843	-0.474488
C	3.173494	3.705527	-1.537273
C	2.901891	2.335905	-1.530350
H	3.250944	1.709902	-2.355703
H	3.724058	4.145901	-2.372206
H	2.961878	5.583379	-0.482211
H	1.716948	4.568226	1.429313
H	1.236926	2.140843	1.447026
H	0.498677	-1.188012	-2.195377
H	1.332319	0.225638	-2.879258
H	-1.172042	0.582679	-2.755565
H	-0.291465	1.769258	-1.785673
C	-1.760047	-1.809551	2.214549
C	-2.240509	-3.265393	2.180399
H	-1.430107	-3.955426	2.479773
C	-2.844052	-3.736769	0.841540
C	-1.886909	-4.369591	-0.178605
C	-0.822852	-3.473729	-0.824356
C	0.269230	-2.957712	0.106983
H	0.498842	-3.694249	0.896815
H	1.209094	-2.769563	-0.439958
H	-0.346501	-4.058798	-1.635222
H	-1.323980	-2.637167	-1.342268
H	-1.377081	-5.228840	0.296315
H	-2.501251	-4.797605	-0.990131
H	-3.613432	-4.495646	1.063449
H	-3.384773	-2.898294	0.369368
H	-3.018345	-3.384420	2.958711
H	-2.599574	-1.155968	1.920248
H	-1.515637	-1.519439	3.256383
C	1.110477	-2.327024	3.354539
C	2.029977	-1.622086	2.671852
H	2.620081	-2.067362	1.865465
H	2.288864	-0.599932	2.963773
H	0.893883	-3.373379	3.122379
H	0.581956	-1.899491	4.211418

^{4}9C-12
Geometry with 89 atoms:
Total energy: -3202.751927430

Cr	0.192721	-1.019258	0.906685
P	1.363853	0.523206	-0.708997
C	1.137309	2.332677	-0.507513
C	1.700013	3.232490	-1.428840
C	1.449091	4.600944	-1.311586
C	0.631990	5.081682	-0.280780
C	0.070769	4.191261	0.638097
C	0.326919	2.821552	0.526630
H	-0.112188	2.133041	1.249772
H	-0.570545	4.560018	1.442113
H	0.434752	6.153045	-0.195134
H	1.892201	5.296794	-2.028198

H	2.343156	2.866291	-2.233393
C	3.123049	0.246318	-1.154568
C	3.418017	-0.550883	-2.275930
C	4.736774	-0.857629	-2.614991
C	5.777035	-0.361959	-1.830188
C	5.493104	0.429277	-0.714615
C	4.177949	0.748471	-0.345086
C	3.907396	1.604503	0.878981
H	2.984940	1.246058	1.358980
C	5.014928	1.658021	1.930214
H	5.914581	2.175189	1.562231
H	4.664856	2.211126	2.815613
H	5.312264	0.649298	2.257349
H	3.674210	2.630178	0.544362
H	6.322813	0.800336	-0.111859
H	6.815467	-0.592636	-2.080473
H	4.944413	-1.481199	-3.487489
H	2.618397	-0.952581	-2.898686
C	0.398939	0.230768	-2.278161
C	-1.060879	0.661825	-2.102212
P	-1.870077	-0.082722	-0.580173
C	-3.041192	1.236768	-0.045746
C	-3.850687	1.807721	-1.051166
C	-4.716667	2.859951	-0.771525
C	-4.783080	3.363935	0.532187
C	-3.998373	2.798279	1.533585
C	-3.121538	1.725627	1.277942
C	-2.364186	1.153055	2.461019
C	-3.265157	0.398144	3.446573
H	-2.683248	0.008159	4.296321
H	-3.777268	-0.447552	2.961502
H	-4.044471	1.059547	3.855077
H	-1.858555	1.975780	2.993864
H	-1.562998	0.479507	2.116321
H	-4.061931	3.194567	2.550827
H	-5.449835	4.197214	0.767163
H	-5.333626	3.287287	-1.565393
H	-3.803066	1.416806	-2.070322
C	-2.956069	-1.404836	-1.251274
C	-2.489329	-2.246148	-2.277384
C	-3.264479	-3.322362	-2.718320
C	-4.511623	-3.575131	-2.139125
C	-4.984964	-2.740124	-1.122119
C	-4.214381	-1.661716	-0.679390
H	-4.604311	-1.009860	0.105891
H	-5.963870	-2.924309	-0.672582
H	-5.115943	-4.417578	-2.483844
H	-2.890819	-3.964641	-3.519568
H	-1.519198	-2.067640	-2.746332
H	-1.123444	1.752748	-1.977833
H	-1.648386	0.401384	-2.995243
H	0.869298	0.797264	-3.097283
H	0.471789	-0.837962	-2.527347
C	0.772374	-2.587256	-0.284806
C	1.230576	-3.888705	0.371251
H	0.560756	-4.182905	1.199434
C	2.688092	-3.926813	0.853435
C	3.048382	-3.184071	2.148171
C	3.033207	-1.646914	2.111282
C	1.666109	-0.998847	2.329119
H	1.230276	-1.374702	3.272814
H	1.777828	0.097095	2.472619
H	3.720706	-1.285374	2.899984
H	3.478193	-1.309653	1.160686
H	2.398681	-3.539390	2.970751
H	4.068041	-3.503193	2.424115
H	2.959398	-4.986871	0.998852
H	3.340738	-3.560875	0.038721
H	1.113734	-4.696816	-0.377375
H	1.553956	-2.238917	-0.980461
H	-0.156201	-2.746096	-0.865513
C	-1.047069	-2.507411	2.847656
C	-1.851775	-2.579325	1.774300
H	-2.723520	-1.930720	1.670583
H	-1.724983	-3.347226	1.005875
H	-1.223223	-1.779387	3.645567
H	-0.229179	-3.214539	3.003359

[4]9C-13
Geometry with 89 atoms:
Total energy: -3202.749625230

Cr	0.242735	-1.017221	1.020578
P	-1.344797	0.235875	-0.490513
C	-2.646262	-0.878694	-1.129551
C	-2.486784	-1.594949	-2.326178
C	-3.449817	-2.526872	-2.721917
C	-4.573295	-2.759745	-1.923477
C	-4.736272	-2.050813	-0.728717
C	-3.779550	-1.114149	-0.331617
H	-3.920328	-0.562161	0.600443
H	-5.614379	-2.225090	-0.102405
H	-5.322590	-3.492103	-2.232979
H	-3.317468	-3.076523	-3.656889
H	-1.609507	-1.440850	-2.958061
C	-2.218180	1.683166	0.232962
C	-1.889487	2.013078	1.560747
C	-2.460251	3.111320	2.201168
C	-3.374877	3.904016	1.505662
C	-3.705309	3.587066	0.187880
C	-3.148411	2.482509	-0.479330
C	-3.594323	2.224726	-1.906474
H	-2.979692	1.449651	-2.379518
C	-5.069906	1.818687	-2.021578
H	-5.346027	1.663689	-3.076626
H	-5.265582	0.881456	-1.479632
H	-5.736762	2.592719	-1.610448
H	-3.426996	3.146565	-2.490182
H	-4.418522	4.217761	-0.349859
H	-3.831011	4.772341	1.987658
H	-2.188445	3.345583	3.232862
H	-1.173394	1.401084	2.107102
C	-0.416652	0.916823	-1.976945
C	1.051134	0.478446	-2.082883
P	1.907640	0.503688	-0.425564
C	3.714606	0.332775	-0.764043
C	4.579065	1.404515	-0.468647
C	5.955671	1.291619	-0.664410
C	6.485844	0.099857	-1.161486
C	5.637027	-0.969887	-1.449921
C	4.248698	-0.885526	-1.257573
C	3.362456	-2.066479	-1.603000
C	3.909753	-3.446867	-1.232998
H	4.180557	-3.501730	-0.166163
H	4.805214	-3.711847	-1.815360
H	3.153187	-4.221969	-1.432338
H	3.147742	-2.043097	-2.687266
H	2.388989	-1.937190	-1.112577
H	6.066536	-1.895537	-1.838019
H	7.561854	-0.000272	-1.324013
H	6.608505	2.135604	-0.429242
H	4.178123	2.341351	-0.079652
C	1.696238	2.240260	0.141611
C	1.643146	3.330173	-0.745591
C	1.446269	4.625760	-0.262686
C	1.313442	4.853222	1.111623
C	1.383178	3.780540	2.003628
C	1.568392	2.482964	1.519518
H	1.616072	1.653997	2.229399
H	1.284504	3.951326	3.078245
H	1.157934	5.867862	1.485919
H	1.400300	5.463413	-0.962898
H	1.762798	3.174980	-1.820189
H	1.127448	-0.556125	-2.448942
H	1.587589	1.111767	-2.806541
H	-0.956894	0.657923	-2.898616
H	-0.482396	2.008308	-1.869765
C	-1.156837	-1.385635	2.458512
C	-1.131902	-2.696282	3.251060
H	-0.101074	-2.968774	3.546299
C	-1.780566	-3.903013	2.563117
C	-1.042626	-4.528594	1.370942
C	-1.032061	-3.730205	0.055823
C	0.092757	-2.715410	-0.116087
H	1.071027	-3.200718	0.062252
H	0.108630	-2.327015	-1.152053
H	-0.950794	-4.454231	-0.778445
H	-2.012869	-3.249023	-0.082368
H	-0.004696	-4.777537	1.664455
H	-1.527263	-5.498460	1.167510
H	-1.908274	-4.691782	3.325001
H	-2.803093	-3.627987	2.243581
H	-1.665125	-2.539863	4.208942
H	-2.174559	-1.202773	2.073137
H	-0.921436	-0.534561	3.136582
C	2.093316	-1.168472	3.024371
C	2.370271	-2.231984	2.252540
H	1.932500	-3.214732	2.450554
H	3.084426	-2.163604	1.425749
H	1.425556	-1.240459	3.887644
H	2.594033	-0.209180	2.858660

[4]9C-14
Geometry with 89 atoms:
Total energy: -3202.748732330

Cr	0.049699	-1.147682	1.129259
P	-1.551412	0.168903	-0.329009
C	-3.161235	-0.549842	-0.816364
C	-3.312258	-1.283246	-2.005311
C	-4.523604	-1.918377	-2.291626
C	-5.592688	-1.832405	-1.394998
C	-5.449592	-1.102045	-0.211078
C	-4.241988	-0.463712	0.079297
H	-4.144971	0.106913	1.005325
H	-6.282424	-1.027240	0.492192
H	-6.537590	-2.332790	-1.619763
H	-4.630044	-2.484462	-3.220027
H	-2.488832	-1.372826	-2.717336
C	-1.948299	1.708592	0.599322
C	-1.485833	1.767747	1.928933
C	-1.641396	2.913511	2.707044
C	-2.268796	4.030436	2.149358
C	-2.752186	3.974199	0.842142
C	-2.621454	2.823941	0.043940
C	-3.240482	2.845827	-1.339949
H	-2.954988	1.956475	-1.914154
C	-4.773386	2.930272	-1.309622
H	-5.206229	2.056723	-0.798673
H	-5.120684	3.835162	-0.786787
H	-5.177399	2.958363	-2.333895
H	-2.838708	3.713688	-1.890961
H	-3.253233	4.849762	0.420583
H	-2.390097	4.944418	2.735949
H	-1.273433	2.934472	3.735258
H	-0.992579	0.900066	2.376485
C	-0.676743	0.705240	-1.897123
C	0.658606	-0.019508	-2.099791
P	1.733515	0.148277	-0.586495
C	3.307144	-0.698828	-1.028178
C	3.381639	-1.522359	-2.166494
C	4.540714	-2.244295	-2.458433
C	5.641961	-2.149318	-1.608219
C	5.579318	-1.332043	-0.476836
C	4.428423	-0.594277	-0.161859
C	4.401667	0.319468	1.048969
C	5.326733	-0.053468	2.206732
H	5.164761	-1.090817	2.541204
H	5.145828	0.610871	3.066129
H	6.389374	0.050191	1.938920
H	3.367147	0.377290	1.421886
H	4.627912	1.347267	0.713455
H	6.452156	-1.268655	0.174801
H	6.554439	-2.710955	-1.823029
H	4.576533	-2.878783	-3.347132
H	2.532218	-1.617731	-2.843379
C	2.126451	1.945148	-0.620334
C	1.553741	2.798785	0.334610
C	1.802856	4.174253	0.295403
C	2.634394	4.705166	-0.694259
C	3.215120	3.858685	-1.646716
C	2.962418	2.485611	-1.613077
H	3.425607	1.831172	-2.356289
H	3.869639	4.270843	-2.418807
H	2.834467	5.779112	-0.724007
H	1.344617	4.828006	1.041509
H	0.900870	2.397160	1.111386
H	0.493127	-1.093527	-2.273262
H	1.182426	0.388884	-2.978395
H	-1.335611	0.543660	-2.762196
H	-0.515998	1.790593	-1.817039
C	-1.470914	-1.923367	2.290398
C	-1.864819	-3.402915	2.197533
H	-1.002109	-4.050732	2.439538
C	-2.482176	-3.855085	0.858971

C	-1.517535	-4.396446	-0.205905
C	-0.509745	-3.421394	-0.825662
C	0.548536	-2.861015	0.120038
H	0.784857	-3.575598	0.927155
H	1.489449	-2.641620	-0.410793
H	0.000923	-3.950590	-1.653720
H	-1.061305	-2.602480	-1.321891
H	-0.957435	-5.248517	0.222482
H	-2.124885	-4.818213	-1.025968
H	-3.204249	-4.662083	1.069718
H	-3.078592	-3.030450	0.433907
H	-2.604161	-3.605944	2.995798
H	-2.371727	-1.302948	2.127216
H	-1.132662	-1.700335	3.321966
C	1.537968	-0.708433	3.252523
C	1.973065	-1.889906	2.781123
H	1.573367	-2.834038	3.163298
H	2.771758	-1.956240	2.035616
H	0.781782	-0.654036	4.041883
H	1.978622	0.239603	2.927190

^{4}9C-15
Geometry with 89 atoms:
Total energy: -3202.749365520

Cr	0.079059	-1.068793	1.036576
P	-1.507468	0.301513	-0.370574
C	-2.742733	-0.793328	-1.158639
C	-2.494034	-1.389825	-2.405287
C	-3.400179	-2.310731	-2.937405
C	-4.558298	-2.646628	-2.230121
C	-4.812984	-2.051200	-0.990253
C	-3.911054	-1.129618	-0.454179
H	-4.124358	-0.665121	0.511018
H	-5.720179	-2.304014	-0.436168
H	-5.264170	-3.369409	-2.646103
H	-3.197596	-2.769800	-3.908030
H	-1.592276	-1.147496	-2.970888
C	-2.433451	1.641687	0.474774
C	-2.134063	1.830888	1.837541
C	-2.760536	2.822956	2.589650
C	-3.713042	3.640073	1.976698
C	-4.016871	3.460014	0.627089
C	-3.391088	2.474904	-0.156446
C	-3.754852	2.405803	-1.626081
H	-4.853827	2.434115	-1.713264
C	-3.161325	3.562253	-2.443534
H	-3.517546	4.536874	-2.074416
H	-2.061600	3.573179	-2.391186
H	-3.450780	3.477782	-3.503186
H	-3.449894	1.446508	-2.063297
H	-4.766273	4.103053	0.157007
H	-4.224007	4.417228	2.550496
H	-2.514719	2.948339	3.646601
H	-1.405819	1.178362	2.320244
C	-0.568187	1.128279	-1.760385
C	0.775660	0.463673	-2.075749
P	1.792471	0.284156	-0.515441
C	3.377399	-0.471341	-1.086993
C	3.210101	-1.561852	-1.968455
C	4.294259	-2.310362	-2.423394
C	5.580894	-1.980742	-1.995585
C	5.757259	-0.916397	-1.112230
C	4.683440	-0.145230	-0.631001
C	4.998298	0.943536	0.376847
C	4.588217	0.585207	1.808701
H	3.504148	0.419680	1.881466
H	4.841580	1.399957	2.505145
H	5.091141	-0.331925	2.153847
H	4.521296	1.889341	0.088830
H	6.082103	1.133927	0.354024
H	6.766840	-0.667258	-0.774173
H	6.445188	-2.551884	-2.343050
H	4.129505	-3.145582	-3.108112
H	2.212032	-1.847737	-2.303378
C	2.010683	2.059994	-0.094386
C	1.574150	2.512939	1.159920
C	1.628123	3.871939	1.485931
C	2.120366	4.790609	0.556444
C	2.556212	4.349548	-0.699873
C	2.499186	2.994012	-1.026033
H	2.849845	2.661592	-2.006603
H	2.942985	5.067220	-1.427504
H	2.163211	5.853319	0.806981
H	1.279755	4.210744	2.464397
H	1.183804	1.803175	1.893924
H	0.630908	-0.533391	-2.513296
H	1.335965	1.059510	-2.812289
H	-1.201867	1.173611	-2.657876
H	-0.408472	2.164438	-1.426685
C	-1.379594	-1.620723	2.371712
C	-1.356879	-3.001538	3.037889
H	-0.345933	-3.253453	3.409989
C	-1.861953	-4.169958	2.183173
C	-0.979662	-4.629876	1.014117
C	-0.959692	-3.734482	-0.236931
C	0.091907	-2.631607	-0.288295
H	1.108856	-3.045208	-0.142429
H	0.075597	-2.158966	-1.284815
H	-0.787191	-4.385478	-1.116597
H	-1.964713	-3.310019	-0.394396
H	0.054046	-4.799136	1.371521
H	-1.346368	-5.623455	0.706065
H	-2.002065	-5.034377	2.855405
H	-2.868670	-3.926635	1.795313
H	-1.988088	-2.964302	3.947128
H	-2.381410	-1.439639	1.944876
H	-1.231221	-0.835189	3.146003
C	1.709764	-1.312716	3.169525
C	2.170560	-2.212408	2.284626
H	1.843758	-3.255890	2.313961
H	2.932091	-1.953211	1.542108
H	1.003814	-1.590875	3.955665
H	2.082106	-0.283014	3.187820

^{4}9C-16
Geometry with 89 atoms:
Total energy: -3202.749433250

Cr	0.305218	-1.140006	-1.147306
P	1.622557	0.356144	0.355255
C	3.379894	0.054671	0.753210
C	4.361765	0.446100	-0.174369
C	5.710706	0.190004	0.078963
C	6.094801	-0.458180	1.257466
C	5.124120	-0.844759	2.185959
C	3.772361	-0.590944	1.938529
H	3.033788	-0.903090	2.678775
H	5.418145	-1.346581	3.110950
H	7.150928	-0.657591	1.454160
H	6.465207	0.501747	-0.647136
H	4.076061	0.967011	-1.091114
C	1.540643	2.063099	-0.328670
C	1.008717	2.166403	-1.630271
C	0.873314	3.396562	-2.270690
C	1.281703	4.554651	-1.605887
C	1.824176	4.463985	-0.323789
C	1.970214	3.234906	0.342911
C	2.557055	3.253264	1.740126
H	3.459522	3.886814	1.724315
C	1.588122	3.801892	2.797884
H	1.282624	4.833514	2.561944
H	0.670492	3.197013	2.866607
H	2.062592	3.811099	3.791967
H	2.905840	2.253801	2.030760
H	2.154475	5.375179	0.182685
H	1.187346	5.529839	-2.089796
H	0.458852	3.448482	-3.279917
H	0.707189	1.262319	-2.168141
C	0.704056	0.354386	1.966465
C	-0.712860	0.894292	1.757947
P	-1.664258	0.046139	0.376515
C	-2.773851	-1.156276	1.239819
C	-2.327499	-1.688240	2.468381
C	-3.035362	-2.687599	3.133852
C	-4.213936	-3.183723	2.573430
C	-4.662935	-2.669189	1.358887
C	-3.968862	-1.661203	0.665173
C	-4.577043	-1.180399	-0.640655
C	-5.896860	-0.420037	-0.456649
H	-6.658138	-1.046668	0.033970
H	-6.299845	-0.102460	-1.431550
H	-5.753863	0.479807	0.159238
H	-4.756045	-2.059513	-1.283194
H	-3.875861	-0.542231	-1.189575
H	-5.584468	-3.062284	0.920563
H	-4.779086	-3.971214	3.077742
H	-2.663252	-3.076551	4.084566
H	-1.405651	-1.327883	2.926627
C	-2.717157	1.442926	-0.184936
C	-2.564983	1.948439	-1.484822
C	-3.310423	3.053710	-1.905678
C	-4.209925	3.664304	-1.027305
C	-4.363992	3.168299	0.272414
C	-3.623699	2.061377	0.692957
H	-3.758132	1.670253	1.704760
H	-5.068738	3.642510	0.959799
H	-4.792903	4.528511	-1.354933
H	-3.186059	3.439509	-2.920417
H	-1.857075	1.483578	-2.174912
H	-1.292550	0.863557	2.692494
H	-0.665004	1.949988	1.452169
H	0.694045	-0.693062	2.306466
H	1.237481	0.941853	2.727049
C	1.909580	-1.379794	-2.421462
C	2.549491	-2.733053	-2.742319
H	1.800722	-3.453213	-3.118529
C	3.335472	-3.390073	-1.596865
C	2.535792	-4.173121	-0.544857
C	1.750013	-3.372794	0.502587
C	0.417662	-2.773938	0.066703
H	-0.191765	-3.526739	-0.469092
H	-0.172369	-2.469349	0.949988
H	1.546625	-4.054269	1.352289
H	2.412402	-2.593911	0.916271
H	1.851116	-4.877283	-1.054819
H	3.254591	-4.806495	0.002965
H	4.049710	-4.098813	-2.050065
H	3.954827	-2.626429	-1.090536
H	3.252453	-2.587932	-3.585337
H	2.705175	-0.695666	-2.079200
H	1.503512	-0.921590	-3.349446
C	-1.816518	-1.983481	-2.416092
C	-0.822208	-2.547825	-3.123649
H	-0.451717	-2.105616	-4.052553
H	-0.386045	-3.506414	-2.832588
H	-2.311293	-1.067789	-2.753940
H	-2.234822	-2.471728	-1.531709

^{4}9C-17
Geometry with 89 atoms:
Total energy: -3202.751034610

Cr	0.096880	-1.014679	0.937006
P	1.288864	0.388631	-0.804368
C	1.121967	2.215017	-0.738127
C	1.658768	3.019640	-1.758245
C	1.473509	4.403035	-1.729527
C	0.748498	4.994783	-0.687642
C	0.212768	4.199808	0.328559
C	0.402677	2.815034	0.304803
H	-0.012589	2.204767	1.106740
H	-0.356001	4.655724	1.142375
H	0.603152	6.077587	-0.669689
H	1.897121	5.023274	-2.523188
H	2.231644	2.567176	-2.572162
C	3.032137	0.030339	-1.262746
C	3.278604	-0.866520	-2.318976
C	4.579771	-1.229185	-2.669858
C	5.653132	-0.690015	-1.962279
C	5.417907	0.199538	-0.911428
C	4.121072	0.578194	-0.532033
C	3.910935	1.551353	0.614418
H	2.983398	1.284085	1.141554
C	5.042514	1.646670	1.637104
H	5.953340	2.095423	1.211333
H	4.733490	2.283598	2.480385
H	5.307689	0.656688	2.039926
H	3.717671	2.552281	0.190772
H	6.273004	0.604144	-0.368868
H	6.678851	-0.962474	-2.222728
H	4.747108	-1.929376	-3.491475
H	2.454767	-1.301602	-2.884504
C	0.293698	0.001627	-2.336380
C	-1.155303	0.470101	-2.168969
P	-1.928162	-0.174668	-0.585413

C -2.993265 1.218862 -0.018433
C -3.835962 1.808552 -0.980804
C -4.635560 2.905116 -0.666511
C -4.595855 3.427334 0.628390
C -3.771113 2.845606 1.591642
C -2.961709 1.732857 1.302145
C -2.130570 1.108579 2.410483
C -1.666914 2.037790 3.531137
H -0.970304 1.507846 4.199398
H -2.504914 2.389677 4.151035
H -1.146260 2.923866 3.134688
H -1.235846 0.637756 1.965966
H -2.700359 0.270400 2.847557
H -3.762690 3.268171 2.597184
H -5.210710 4.291238 0.892774
H -5.281454 3.349330 -1.427317
H -3.868497 1.400332 -1.994090
C -3.094798 -1.475200 -1.144272
C -2.641785 -2.449059 -2.053375
C -3.469883 -3.513052 -2.419320
C -4.754207 -3.623449 -1.876012
C -5.209440 -2.660632 -0.970476
C -4.386617 -1.591281 -0.604081
H -4.760703 -0.840360 0.095572
H -6.214692 -2.736909 -0.548680
H -5.400095 -4.457331 -2.160973
H -3.108757 -4.259493 -3.130982
H -1.639294 -2.381812 -2.483370
H -1.199045 1.567911 -2.117539
H -1.764692 0.156785 -3.029856
H 0.761080 0.491451 -3.204903
H 0.337663 -1.084872 -2.503113
C 0.708585 -2.686414 -0.077099
C 1.210728 -3.890651 0.717142
H 0.526056 -4.137030 1.549117
C 2.650248 -3.805898 1.245579
C 2.930611 -2.928874 2.475717
C 2.892303 -1.402864 2.282715
C 1.513184 -0.752742 2.407438
H 1.085561 -0.995217 3.396598
H 1.607271 0.353672 2.388114
H 3.560882 -0.950645 3.040330
H 3.352206 -1.161862 1.310481
H 2.250565 -3.216683 3.299973
H 3.941735 -3.195084 2.827981
H 2.966386 -4.832670 1.498779
H 3.313350 -3.484796 0.420600
H 1.160529 -4.773044 0.049206
H 1.466523 -2.406009 -0.828164
H -0.223057 -2.937654 -0.619592
C -1.100888 -2.255261 2.920553
C -1.958236 -2.393391 1.893446
H -2.821931 -1.733817 1.779954
H -1.887635 -3.223801 1.184932
H -1.228273 -1.467175 3.668437
H -0.297957 -2.972704 3.099942

^{49}C-18
Geometry with 89 atoms:
Total energy: -3202.747892720
Cr 0.029286 -1.188254 1.134012
P -1.527037 0.207572 -0.309328
C -3.126924 -0.498179 -0.850225
C -3.249884 -1.198970 -2.062201
C -4.456646 -1.817340 -2.399592
C -5.550501 -1.746773 -1.531939
C -5.436363 -1.047668 -0.326415
C -4.233140 -0.425918 0.014655
H -4.161812 0.124151 0.955250
H -6.288748 -0.983169 0.354053
H -6.491960 -2.233976 -1.796520
H -4.540034 -2.357935 -3.345410
H -2.408361 -1.275070 -2.754398
C -1.944373 1.724392 0.645815
C -1.526074 1.745401 1.991253
C -1.709930 2.868252 2.796028
C -2.319513 4.000577 2.249664
C -2.757924 3.982080 0.925712
C -2.600191 2.854719 0.100184
C -3.176140 2.915142 -1.301201
H -2.873462 2.041949 -1.890862
C -4.709261 3.000793 -1.316062
H -5.072079 3.889639 -0.776511
H -5.081033 3.061382 -2.351091
H -5.158548 2.112399 -0.846470
H -2.757162 3.797197 -1.815639
H -3.245523 4.869283 0.512633
H -2.461814 4.897256 2.857865
H -1.377143 2.859682 3.836312
H -1.046550 0.864322 2.427909
C -0.626013 0.764549 -1.853674
C 0.687649 0.004174 -2.059767
P 1.757715 0.144869 -0.538235
C 3.340985 -0.673511 -1.001582
C 3.370402 -1.572191 -2.085558
C 4.531046 -2.277079 -2.407915
C 5.683058 -2.087815 -1.644702
C 5.664442 -1.199182 -0.567782
C 4.510994 -0.478763 -0.219567
C 4.547748 0.503446 0.937314
C 5.454579 0.128866 2.110500
H 5.219155 -0.875296 2.498973
H 5.327768 0.850321 2.933023
H 6.520691 0.140674 1.837574
H 3.526573 0.654223 1.315499
H 4.841327 1.492941 0.543700
H 6.576501 -1.062909 0.015572
H 6.599908 -2.631727 -1.885026
H 4.529765 -2.970060 -3.252534
H 2.480949 -1.741659 -2.692915
C 2.105830 1.951608 -0.545914
C 1.541056 2.768139 0.444980
C 1.743139 4.151637 0.423008
C 2.521183 4.726940 -0.585242
C 3.096138 3.916952 -1.572367
C 2.889208 2.535845 -1.556303
H 3.347714 1.910409 -2.326982
H 3.709972 4.364237 -2.358192
H 2.685028 5.807261 -0.602075
H 1.290272 4.776552 1.196543
H 0.932915 2.329632 1.238076
H 0.492031 -1.062975 -2.243115
H 1.228773 0.403878 -2.931852
H -1.281355 0.644250 -2.727917
H -0.434555 1.842132 -1.742682
C -1.575866 -1.909791 2.218069
C -1.959928 -3.392994 2.171846
H -1.101519 -4.033080 2.448239
C -2.557794 -3.885253 0.838427
C -1.580292 -4.437574 -0.208721
C -0.597964 -3.459269 -0.863615
C 0.467219 -2.867937 0.053543
H 0.761739 -3.589448 0.836049
H 1.382520 -2.614998 -0.507266
H -0.091497 -4.000778 -1.686457
H -1.171003 -2.661078 -1.367170
H -1.000862 -5.263263 0.245351
H -2.179047 -4.899430 -1.013292
H -3.270385 -4.696791 1.063690
H -3.162003 -3.077848 0.389832
H -2.713009 -3.571994 2.962899
H -2.462496 -1.310330 1.945080
H -1.336488 -1.617589 3.260562
C 1.335143 -2.174703 3.284224
C 2.250929 -1.492641 2.574108
H 2.810110 -1.950333 1.752459
H 2.532682 -0.472236 2.849409
H 1.093841 -3.219420 3.069837
H 0.839015 -1.728662 4.151226

^{49}C-19
Geometry with 89 atoms:
Total energy: -3202.749645560
Cr 0.175734 -1.068400 0.883428
P 1.323348 0.513245 -0.720330
C 1.076202 2.323648 -0.553084
C 1.586919 3.204110 -1.522131
C 1.348529 4.575526 -1.414689
C 0.597970 5.078094 -0.344427
C 0.090383 4.206614 0.622579
C 0.332950 2.833845 0.519281
H -0.054914 2.158005 1.281481
H -0.495028 4.594476 1.459608
H 0.412361 6.151977 -0.264715
H 1.751869 5.256825 -2.167848
H 2.183174 2.821687 -2.354834
C 3.089386 0.264988 -1.150796
C 3.413729 -0.528053 -2.266620
C 4.742127 -0.817479 -2.582359
C 5.761385 -0.310304 -1.777527
C 5.447979 0.481576 -0.670115
C 4.122679 0.788851 -0.327167
C 3.818895 1.664747 0.876388
H 2.891096 1.307452 1.350265
C 4.909601 1.755671 1.942468
H 5.808202 2.275002 1.575127
H 4.540361 2.324935 2.809526
H 5.213792 0.758619 2.297331
H 3.578377 2.679588 0.515203
H 6.262813 0.865685 -0.055509
H 6.806815 -0.530091 -2.007636
H 4.973348 -1.437933 -3.451181
H 2.630217 -0.939901 -2.903176
C 0.367527 0.179482 -2.291239
C -1.104405 0.576457 -2.132423
P -1.893246 -0.123931 -0.579253
C -3.085695 1.198381 -0.103471
C -3.923947 1.688542 -1.128007
C -4.792159 2.752141 -0.904013
C -4.830007 3.349983 0.360866
C -4.019074 2.862310 1.381924
C -3.142611 1.777127 1.184606
C -2.346839 1.291447 2.380088
C -3.221824 0.742673 3.514015
H -2.601662 0.387432 4.352103
H -3.851439 -0.093638 3.173648
H -3.894670 1.518809 3.909769
H -1.743788 2.126732 2.773684
H -1.630513 0.515142 2.064069
H -4.061595 3.331746 2.368394
H -5.495774 4.195529 0.550640
H -5.431767 3.116880 -1.711066
H -3.894329 1.225292 -2.117306
C -2.946217 -1.511090 -1.158728
C -2.454018 -2.410516 -2.121806
C -3.202010 -3.532835 -2.487740
C -4.443709 -3.776143 -1.891752
C -4.939142 -2.886758 -0.933300
C -4.197432 -1.759842 -0.567617
H -4.604695 -1.062685 0.168645
H -5.913054 -3.065071 -0.470718
H -5.026226 -4.655188 -2.177608
H -2.811355 -4.220469 -3.241846
H -1.483863 -2.243039 -2.595561
H -1.196456 1.669361 -2.048551
H -1.683276 0.266643 -3.015719
H 0.829390 0.747766 -3.113977
H 0.464218 -0.888648 -2.534410
C 0.904598 -2.621614 -0.263286
C 1.645161 -3.829462 0.309333
H 1.072107 -4.312586 1.118268
C 3.082704 -3.587237 0.792514
C 3.270216 -2.961071 2.181897
C 2.971582 -1.462479 2.320821
C 1.498001 -1.079688 2.420724
H 1.001211 -1.682475 3.207538
H 1.393259 -0.014598 2.730749
H 3.494362 -1.098162 3.226295
H 3.448880 -0.939155 1.477927
H 2.678143 -3.529132 2.924774
H 4.325198 -3.115046 2.466862
H 3.593405 -4.565538 0.804525
H 3.623098 -2.977949 0.044187
H 1.690968 -4.591892 -0.493322
H 1.542905 -2.175107 -1.042865
H -0.039029 -2.938272 -0.749466
C -1.842630 -2.102321 2.390737
C -1.213194 -3.204638 1.957061
H -1.549832 -3.742795 1.065992
H -0.376804 -3.636269 2.511355
H -2.731126 -1.720881 1.882848
H -1.549187 -1.605286 3.319952

^{4}9C-20
Geometry with 89 atoms:
Total energy: -3202.748359680
Cr -0.086676 -1.261040 1.092534
P -1.563240 0.243964 -0.308662
C -3.184777 -0.376005 -0.890279
C -3.308560 -1.054017 -2.115198
C -4.534191 -1.607875 -2.493284
C -5.646533 -1.493146 -1.654285
C -5.531595 -0.814121 -0.437362
C -4.309036 -0.257970 -0.054364
H -4.235406 0.275525 0.895507
H -6.398869 -0.714576 0.219662
H -6.603410 -1.929389 -1.950573
H -4.618248 -2.132046 -3.448269
H -2.452573 -1.161702 -2.785074
C -1.941779 1.730217 0.711445
C -1.622383 1.636333 2.081194
C -1.844266 2.696429 2.958116
C -2.407886 3.876718 2.466668
C -2.744992 3.973617 1.117048
C -2.527302 2.918930 0.212485
C -2.919314 3.138877 -1.234743
H -3.963884 3.492505 -1.256727
C -2.033123 4.169108 -1.950384
H -0.971122 3.877002 -1.936815
H -2.342275 4.285704 -3.001125
H -2.102313 5.157297 -1.469191
H -2.921825 2.191110 -1.789015
H -3.200677 4.895509 0.745278
H -2.596209 4.718523 3.137552
H -1.587550 2.597813 4.015264
H -1.196909 0.711607 2.481466
C -0.629117 0.812415 -1.825408
C 0.654724 0.006429 -2.044996
P 1.702109 0.059710 -0.499741
C 3.277732 -0.768394 -0.967108
C 3.304812 -1.625883 -2.084158
C 4.457958 -2.334924 -2.422641
C 5.605674 -2.189922 -1.643149
C 5.588500 -1.344088 -0.532528
C 4.441012 -0.622957 -0.165173
C 4.483664 0.307549 1.034124
C 5.329995 -0.163613 2.218655
H 5.030765 -1.169925 2.554030
H 5.210819 0.527331 3.068101
H 6.404327 -0.195538 1.982308
H 3.460103 0.494906 1.387758
H 4.839704 1.296668 0.694211
H 6.497579 -1.242113 0.062540
H 6.517746 -2.735799 -1.896812
H 4.454997 -2.995366 -3.292927
H 2.418661 -1.757428 -2.705449
C 2.076412 1.859809 -0.428509
C 1.513493 2.639463 0.592504
C 1.720023 4.022121 0.624237
C 2.501469 4.632903 -0.360384
C 3.077207 3.859100 -1.375850
C 2.865653 2.478997 -1.413130
H 3.323192 1.882106 -2.206685
H 3.694813 4.334034 -2.142228
H 2.667703 5.712702 -0.336462
H 1.266843 4.618474 1.419729
H 0.901250 2.172801 1.365868
H 0.422916 -1.045257 -2.270449
H 1.223290 0.417700 -2.893775
H -1.283530 0.755430 -2.706905
H -0.386127 1.872442 -1.673612
C -1.736153 -1.951916 2.131627
C -2.165436 -3.420058 2.029205
H -1.331737 -4.095940 2.294632
C -2.756419 -3.844844 0.669532
C -1.780761 -4.407369 -0.373942
C -0.748692 -3.451591 -0.983959
C 0.317985 -2.921788 -0.030749
H 0.572695 -3.675024 0.735471
H 1.251703 -2.684124 -0.567870
H -0.244360 -3.992667 -1.808471
H -1.280193 -2.621364 -1.481065
H -1.242786 -5.266845 0.068398
H -2.380766 -4.824047 -1.201918
H -3.508202 -4.630812 0.854292
H -3.315261 -2.998196 0.234248
H -2.936187 -3.602435 2.802232
H -2.601255 -1.317709 1.869349
H -1.498614 -1.703321 3.185907
C 1.165096 -2.407247 3.237210
C 2.068886 -1.679761 2.557276
H 2.641357 -2.095194 1.722410
H 2.332561 -0.667619 2.877662
H 0.940813 -3.444984 2.975525
H 0.655785 -2.007076 4.118796

^{4}9C-21
Geometry with 89 atoms:
Total energy: -3202.748547250
Cr -0.057212 -1.249012 1.092903
P -1.574514 0.206740 -0.323441
C -3.195684 -0.432199 -0.882884
C -3.328844 -1.123842 -2.099021
C -4.552196 -1.699189 -2.451845
C -5.652349 -1.593040 -1.595845
C -5.527509 -0.901924 -0.386626
C -4.307411 -0.324213 -0.028997
H -4.224637 0.215773 0.916517
H -6.384910 -0.810614 0.284451
H -6.607223 -2.046390 -1.872274
H -4.643812 -2.234072 -3.400175
H -2.481117 -1.228830 -2.779752
C -1.959283 1.699029 0.687679
C -1.624501 1.623399 2.054999
C -1.843868 2.692118 2.922175
C -2.421519 3.862661 2.423908
C -2.775570 3.940934 1.077428
C -2.560394 2.877486 0.182609
C -2.973374 3.076487 -1.261863
H -4.024326 3.411253 -1.274739
C -2.114216 4.114709 -1.998489
H -1.046111 3.845405 -1.988112
H -2.433011 4.209398 -3.048553
H -2.200982 5.108354 -1.531543
H -2.965551 2.123310 -1.806618
H -3.243105 4.854786 0.700559
H -2.607851 4.711068 3.086973
H -1.573858 2.607705 3.977248
H -1.188184 0.707572 2.463564
C -0.653864 0.778672 -1.848735
C 0.652162 0.006918 -2.066499
P 1.702070 0.078714 -0.525844
C 3.282157 -0.744606 -0.989067
C 3.363463 -1.514850 -2.164997
C 4.533183 -2.199262 -2.498022
C 5.642905 -2.115093 -1.656115
C 5.571262 -1.354511 -0.487761
C 4.404253 -0.663919 -0.124291
C 4.386425 0.166762 1.146326
C 5.030093 -0.485367 2.372976
H 4.904795 0.157138 3.258719
H 6.110946 -0.645020 2.241956
H 4.574369 -1.463064 2.596010
H 3.348442 0.434653 1.392247
H 4.878598 1.133884 0.939423
H 6.449845 -1.294711 0.157849
H 6.567020 -2.641515 -1.907343
H 4.573883 -2.792197 -3.414777
H 2.510684 -1.593878 -2.839769
C 2.088365 1.877405 -0.466262
C 1.489801 2.677103 0.519046
C 1.711337 4.057696 0.542135
C 2.542605 4.646822 -0.414498
C 3.152698 3.853406 -1.393921
C 2.926991 2.475350 -1.422959
H 3.411641 1.863246 -2.188250
H 3.808644 4.311252 -2.138575
H 2.720728 5.724867 -0.396573
H 1.231575 4.669432 1.309952
H 0.837287 2.229081 1.270062
H 0.450199 -1.050911 -2.291501
H 1.206714 0.434911 -2.916447
H -1.308439 0.694295 -2.728090
H -0.438968 1.846877 -1.711438
C -1.642463 -2.013320 2.172904
C -2.067357 -3.476992 2.001557
H -1.227055 -4.158203 2.230611
C -2.662837 -3.844976 0.627548
C -1.688843 -4.368084 -0.438016
C -0.635241 -3.399189 -0.988395
C 0.419709 -2.922205 0.006303
H 0.620759 -3.689740 0.773305
H 1.377349 -2.697287 -0.492880
H -0.123655 -3.905121 -1.830355
H -1.148534 -2.539159 -1.455120
H -1.167210 -5.257202 -0.037054
H -2.288554 -4.731418 -1.291020
H -3.416619 -4.635831 0.780606
H -3.220465 -2.981167 0.227839
H -2.830812 -3.699951 2.771194
H -2.524246 -1.367805 2.006857
H -1.334966 -1.839920 3.223954
C 1.408742 -0.976038 3.232033
C 1.640532 -2.245631 2.854302
H 1.008231 -3.068381 3.201773
H 2.497399 -2.511840 2.228221
H 0.588278 -0.724413 3.912041
H 2.080399 -0.162189 2.945703

^{4}9C-22
Geometry with 89 atoms:
Total energy: -3202.744389520
Cr -0.251046 -1.459790 1.014644
P -1.453927 0.315221 -0.350602
C -3.154993 -0.008703 -0.953298
C -3.392988 -0.606543 -2.202933
C -4.695437 -0.927499 -2.594517
C -5.772483 -0.657596 -1.745213
C -5.543329 -0.058128 -0.502892
C -4.243807 0.264882 -0.106605
H -4.081378 0.741664 0.862171
H -6.380805 0.162565 0.163244
H -6.790004 -0.910022 -2.052937
H -4.867029 -1.391158 -3.568907
H -2.568915 -0.830260 -2.883509
C -1.602482 1.814049 0.713992
C -1.269756 1.648421 2.073585
C -1.343269 2.704367 2.979751
C -1.766500 3.957004 2.528723
C -2.111236 4.129565 1.188698
C -2.043193 3.079819 0.255337
C -2.434710 3.386044 -1.176747
H -3.437881 3.844955 -1.166516
C -1.459129 4.340867 -1.880120
H -0.435619 3.934833 -1.908022
H -1.779953 4.530131 -2.916688
H -1.405594 5.311765 -1.363296
H -2.545082 2.463555 -1.761443
H -2.454092 5.110183 0.847558
H -1.837683 4.797855 3.223121
H -1.079982 2.547757 4.028260
H -0.950310 0.671223 2.444571
C -0.427962 0.782324 -1.845901
C 0.802681 -0.115023 -2.011759
P 1.805334 -0.117388 -0.430061
C 3.359330 -1.015857 -0.868731
C 3.245005 -2.048791 -1.822867
C 4.324341 -2.869302 -2.151314
C 5.552797 -2.667569 -1.523552
C 5.682401 -1.642819 -0.585596
C 4.614616 -0.798802 -0.232405
C 4.893791 0.289981 0.789434
C 4.206932 0.109541 2.146084
H 3.112346 0.149484 2.056372
H 4.504402 0.914786 2.836074
H 4.474228 -0.853815 2.608371
H 4.619177 1.270813 0.374953
H 5.981737 0.328985 0.950661
H 6.651700 -1.481215 -0.106057
H 6.411027 -3.298993 -1.765871
H 4.200140 -3.658399 -2.896787
H 2.297559 -2.226574 -2.332325
C 2.232106 1.671553 -0.344473
C 1.856394 2.432833 0.770840
C 2.123994 3.805194 0.814575
C 2.771087 4.425049 -0.256892

C 3.154452 3.670616 -1.373560
C 2.885945 2.301784 -1.418981
H 3.203512 1.717866 -2.286946
H 3.667825 4.151607 -2.209790
H 2.981029 5.496983 -0.224427
H 1.820937 4.387521 1.687806
H 1.347856 1.961554 1.612771
H 0.498184 -1.147750 -2.233760
H 1.423420 0.234114 -2.851410
H -1.056835 0.749373 -2.746442
H -0.116156 1.826216 -1.714471
C -1.967972 -1.823024 2.095324
C -2.622218 -3.204697 2.034437
H -1.892549 -3.999749 2.275263
C -3.324828 -3.541680 0.704027
C -2.490185 -4.246330 -0.374525
C -1.383390 -3.445625 -1.073257
C -0.175653 -3.084084 -0.218060
H 0.094950 -3.918636 0.451292
H 0.713530 -2.875008 -0.838263
H -1.034806 -4.049388 -1.934173
H -1.825584 -2.540969 -1.522515
H -2.043448 -5.161005 0.059311
H -3.187211 -4.597278 -1.155365
H -4.175572 -4.206833 0.929354
H -3.771368 -2.623290 0.283453
H -3.380335 -3.257954 2.839318
H -2.722478 -1.057693 1.844903
H -1.635995 -1.595223 3.129475
C 0.783494 -3.110556 2.996828
C 1.619137 -2.115640 2.651772
H 2.401737 -2.256302 1.900758
H 1.618812 -1.162893 3.192664
H 0.835741 -4.092655 2.519210
H 0.052932 -2.999024 3.802213

^{49}C-23
Geometry with 89 atoms:
Total energy: -3202.744493680
Cr 0.029091 -1.296903 0.899861
P -1.395815 0.180385 -0.522973
C -3.049515 -0.439227 -1.010633
C -3.282210 -1.076258 -2.240725
C -4.538432 -1.615613 -2.530360
C -5.572574 -1.535345 -1.593776
C -5.348315 -0.904423 -0.366295
C -4.096886 -0.357427 -0.075379
H -3.944145 0.147610 0.880578
H -6.152578 -0.832276 0.369744
H -6.552527 -1.961659 -1.820944
H -4.705931 -2.104778 -3.492884
H -2.490233 -1.166256 -2.986287
C -1.691331 1.756342 0.381257
C -1.077159 1.872292 1.643085
C -1.177829 3.036335 2.400132
C -1.901746 4.116006 1.889573
C -2.512470 4.013628 0.640125
C -2.432099 2.846637 -0.140027
C -3.144194 2.844654 -1.480841
H -2.907865 1.940817 -2.055325
C -4.670177 2.961774 -1.366217
H -4.970325 3.890662 -0.856761
H -5.131981 2.963888 -2.366172
H -5.089769 2.115790 -0.801842
H -2.761477 3.693831 -2.073937
H -3.070603 4.868357 0.248494
H -1.985068 5.043147 2.461883
H -0.683474 3.103542 3.371205
H -0.488497 1.042615 2.043814
C -0.492629 0.680912 -2.086811
C 1.010209 0.347385 -2.110372
P 1.878845 0.242777 -0.464179
C 3.626103 -0.039418 -1.025055
C 4.302579 1.065122 -1.585079
C 5.585450 0.937170 -2.109766
C 6.214828 -0.311459 -2.085782
C 5.558091 -1.405320 -1.528320
C 4.264114 -1.301111 -0.982208
C 3.629881 -2.544781 -0.393303
C 4.461615 -3.219268 0.704557
H 4.628430 -2.542083 1.557464
H 5.450141 -3.536266 0.339524
H 3.953005 -4.122277 1.078079
H 3.447198 -3.270034 -1.205706
H 2.641087 -2.294198 0.006687
H 6.058201 -2.376801 -1.519643
H 7.218476 -0.431568 -2.501281
H 6.090175 1.806784 -2.537230
H 3.819216 2.043918 -1.607602
C 1.942661 1.955094 0.201367
C 1.417186 3.074997 -0.461707
C 1.479071 4.341142 0.128318
C 2.075523 4.507266 1.380330
C 2.612747 3.399313 2.044790
C 2.540488 2.133076 1.462632
H 2.968346 1.276712 1.989605
H 3.089233 3.521911 3.020581
H 2.123760 5.498296 1.837709
H 1.057284 5.201354 -0.396779
H 0.955610 2.978150 -1.444422
H 1.172847 -0.654310 -2.538711
H 1.547564 1.051563 -2.764546
H -0.984850 0.203590 -2.945053
H -0.651750 1.760983 -2.200183
C -1.503231 -1.712263 2.193595
C -1.958258 -3.143423 2.491127
H -1.105904 -3.779181 2.793730
C -2.720659 -3.854334 1.361769
C -1.883002 -4.532900 0.267868
C -1.207806 -3.638927 -0.780002
C 0.056648 -2.900424 -0.356572
H 0.745509 -3.584834 0.176887
H 0.596631 -2.521434 -1.244650
H -0.944265 -4.284281 -1.641306
H -1.954136 -2.930622 -1.173780
H -1.119998 -5.178911 0.743135
H -2.553677 -5.219969 -0.276206
H -3.341590 -4.640331 1.824589
H -3.431240 -3.147659 0.895716
H -2.621543 -3.114194 3.377200
H -2.384158 -1.108335 1.920076
H -1.088715 -1.244452 3.113654
C 1.995126 -1.331024 2.729491
C 1.556405 -2.599248 2.795739
H 0.718497 -2.885201 3.434982
H 2.060383 -3.405553 2.256763
H 1.534340 -0.533704 3.323643
H 2.887505 -1.065860 2.156978

^{49}C-24
Geometry with 89 atoms:
Total energy: -3202.745727470
Cr 0.077716 -1.216368 1.017994
P -1.353482 0.167262 -0.511994
C -3.001438 -0.477637 -0.990335
C -3.228052 -1.165249 -2.193515
C -4.487015 -1.703683 -2.473317
C -5.530054 -1.571806 -1.552582
C -5.311905 -0.890551 -0.351135
C -4.057951 -0.344041 -0.070999
H -3.910328 0.202922 0.862339
H -6.123023 -0.777628 0.372095
H -6.512362 -1.996687 -1.772153
H -4.650221 -2.231728 -3.415815
H -2.428753 -1.295088 -2.925103
C -1.691107 1.789845 0.292468
C -1.173988 1.959292 1.590764
C -1.303475 3.163809 2.277413
C -1.959501 4.229692 1.658033
C -2.488334 4.068877 0.377709
C -2.381550 2.859128 -0.330829
C -3.034532 2.788849 -1.699416
H -2.760436 1.868023 -2.227581
C -4.566234 2.875247 -1.643788
H -4.903114 3.808941 -1.167051
H -4.991361 2.842945 -2.659391
H -4.985853 2.033214 -1.073756
H -2.647216 3.621981 -2.311569
H -3.004099 4.908666 -0.096060
H -2.060149 5.188476 2.172490
H -0.885823 3.271035 3.280534
H -0.655938 1.132773 2.082534
C -0.425539 0.578629 -2.089617
C 1.076930 0.240282 -2.078800
P 1.904834 0.208819 -0.411144
C 3.674573 -0.093057 -0.871827
C 4.388589 0.987353 -1.431653
C 5.719702 0.851387 -1.815975
C 6.366956 -0.375323 -1.632885
C 5.670602 -1.446613 -1.079543
C 4.320541 -1.338211 -0.695658
C 3.634216 -2.576005 -0.162713
C 3.341652 -3.614488 -1.253409
H 4.271428 -3.962707 -1.730154
H 2.703098 -3.193441 -2.046184
H 2.824621 -4.492304 -0.835547
H 2.699173 -2.295500 0.335897
H 4.275222 -3.035348 0.609269
H 6.179926 -2.403786 -0.936581
H 7.415182 -0.493930 -1.918341
H 6.252707 1.701634 -2.247994
H 3.898819 1.955065 -1.558409
C 1.943100 1.949430 0.184491
C 2.515008 2.185544 1.448813
C 2.559722 3.474657 1.981219
C 2.023194 4.548789 1.263065
C 1.455597 4.325660 0.006667
C 1.420108 3.036273 -0.533262
H 0.982676 2.896312 -1.521802
H 1.035631 5.158912 -0.561454
H 2.050283 5.557597 1.681625
H 3.015750 3.641364 2.960265
H 2.946811 1.359405 2.018699
H 1.244232 -0.778302 -2.463144
H 1.627538 0.917851 -2.749899
H -0.910513 0.060539 -2.928136
H -0.577342 1.651765 -2.260828
C -1.462506 -1.575653 2.319720
C -1.950284 -2.985587 2.665330
H -1.114568 -3.625124 3.004524
C -2.712128 -3.726231 1.554191
C -1.872555 -4.476596 0.510326
C -1.161025 -3.647152 -0.564914
C 0.090418 -2.886924 -0.145228
H 0.766186 -3.544656 0.434762
H 0.648895 -2.552052 -1.037732
H -0.869436 -4.342899 -1.376833
H -1.892148 -2.964318 -1.025892
H -1.131602 -5.114046 1.029950
H -2.547984 -5.175254 -0.012813
H -3.364724 -4.472052 2.039298
H -3.392216 -3.022328 1.040906
H -2.624165 -2.909346 3.540443
H -2.331464 -0.964063 2.023322
H -1.046684 -1.086765 3.228628
C 2.004988 -1.209702 2.870034
C 1.600054 -2.487718 2.957985
H 0.748659 -2.782957 3.575163
H 2.144121 -3.291915 2.454267
H 1.505267 -0.409850 3.428282
H 2.909148 -0.936817 2.319165

^{41}0A-01
Geometry with 77 atoms:
Total energy: -3045.618980020
Cr 0.208523 -0.727746 0.946585
C -0.033485 -2.543784 0.027722
C -1.355492 -3.304448 0.179355
C -1.668886 -3.933023 1.548911
C -2.307750 -2.996765 2.586562
C -1.439026 -1.822265 3.036524
C -0.167951 -2.198706 3.805812
C 0.902517 -1.103269 3.809083
C 1.600332 -0.960093 2.445574
H 2.186865 -1.866617 2.209155
H 2.310137 -0.112224 2.451867
H 1.648258 -1.327498 4.595135
H 0.442080 -0.142897 4.114531
H 0.272923 -3.115944 3.381613
H -0.470148 -2.452844 4.835703
H -2.034615 -1.113598 3.636762
H -1.242288 -1.213597 2.112795
H -2.579166 -3.580889 3.483472

H	-3.255685	-2.606481	2.176380
H	-0.755834	-4.397771	1.959752
H	-2.375089	-4.764301	1.389072
H	-2.203399	-2.668332	-0.128697
H	-1.341432	-4.125269	-0.563170
H	0.823547	-3.140844	0.389351
H	0.145860	-2.322392	-1.041179
P	1.846291	0.179336	-0.626681
C	3.384097	-0.746564	-0.934578
C	3.375453	-1.860508	-1.793581
C	4.530860	-2.627251	-1.959527
C	5.699018	-2.298563	-1.264525
C	5.709032	-1.200135	-0.399570
C	4.558145	-0.426817	-0.229691
H	4.580168	0.428734	0.448745
H	6.618471	-0.940695	0.147740
H	6.601665	-2.899937	-1.396354
H	4.516776	-3.486563	-2.634240
H	2.470177	-2.142591	-2.335685
C	2.283690	1.888949	-0.164330
C	3.218585	2.649572	-0.886998
C	3.445387	3.982904	-0.540023
C	2.738248	4.566189	0.519050
C	1.805791	3.815072	1.240566
C	1.585408	2.477887	0.901807
H	0.863529	1.880463	1.468728
H	1.252763	4.267253	2.066926
H	2.918162	5.611182	0.782997
H	4.176496	4.571994	-1.098942
H	3.773774	2.199295	-1.713998
C	0.981910	0.376852	-2.262673
C	-0.322123	1.170762	-2.092894
P	-1.419817	0.518309	-0.718240
C	-2.718380	-0.461240	-1.559613
C	-2.403929	-1.265084	-2.668774
C	-3.369099	-2.111100	-3.221350
C	-4.653084	-2.168323	-2.671119
C	-4.971956	-1.370305	-1.567570
C	-4.011627	-0.521912	-1.011397
H	-4.274368	0.098843	-0.151084
H	-5.976069	-1.405232	-1.137808
H	-5.405440	-2.832335	-3.103309
H	-3.114622	-2.729744	-4.085417
H	-1.403421	-1.247967	-3.106532
C	-2.273990	2.002686	-0.071732
C	-2.853407	2.952237	-0.932248
C	-3.478658	4.084485	-0.407742
C	-3.536843	4.277946	0.977915
C	-2.970033	3.335941	1.840306
C	-2.339425	2.202526	1.316871
H	-1.904879	1.468791	2.002138
H	-3.017922	3.482116	2.922054
H	-4.028594	5.164936	1.384730
H	-3.925929	4.818863	-1.082016
H	-2.820854	2.804618	-2.014590
H	-0.095105	2.213602	-1.823101
H	-0.887561	1.195127	-3.036600
H	1.657732	0.882301	-2.970797
H	0.791395	-0.633453	-2.657103

H	-3.520780	-2.355816	2.122197
H	-1.093381	-4.228572	1.867190
H	-2.741638	-4.538519	1.356078
H	-2.530708	-2.428218	-0.168911
H	-1.805949	-3.947641	-0.644215
H	0.455829	-3.170338	0.186666
H	-0.192976	-2.239836	-1.184131
P	1.791429	0.184304	-0.601514
C	2.927017	-0.958470	-1.467085
C	3.690564	-0.517423	-2.563822
C	4.586088	-1.385596	-3.189996
C	4.734298	-2.697483	-2.725087
C	3.988276	-3.137641	-1.628900
C	3.087562	-2.272983	-0.999767
H	2.513305	-2.623535	-0.142390
H	4.104552	-4.159054	-1.259068
H	5.436148	-3.375138	-3.217268
H	5.174362	-1.035031	-4.041426
H	3.602789	0.508877	-2.927786
C	2.858077	1.370749	0.302468
C	4.199770	1.074770	0.593239
C	4.960786	1.960809	1.361712
C	4.392714	3.141163	1.849222
C	3.053920	3.436211	1.569812
C	2.287411	2.554890	0.805416
H	1.241276	2.800277	0.603847
H	2.602223	4.356663	1.947872
H	4.992321	3.831256	2.447653
H	6.005859	1.725740	1.577489
H	4.657055	0.156968	0.218192
C	0.943488	1.197341	-1.926328
C	-0.458654	0.667517	-2.251269
P	-1.499803	0.604952	-0.711347
C	-3.139767	-0.024832	-1.222374
C	-4.194662	0.075640	-0.295934
C	-5.442329	-0.477512	-0.585396
C	-5.650787	-1.142064	-1.799917
C	-4.608948	-1.242025	-2.724935
C	-3.356426	-0.687087	-2.441016
H	-2.557660	-0.781840	-3.178451
H	-4.768206	-1.754858	-3.676673
H	-6.626606	-1.579299	-2.024470
H	-6.255292	-0.391811	0.139763
H	-4.041336	0.591154	0.656728
C	-1.782843	2.367050	-0.282944
C	-1.496611	2.808626	1.019415
C	-1.696738	4.146915	1.375183
C	-2.184122	5.052260	0.429518
C	-2.478431	4.619132	-0.869683
C	-2.283076	3.283674	-1.225035
H	-2.530133	2.951762	-2.237026
H	-2.867756	5.325997	-1.606440
H	-2.341531	6.098055	0.704553
H	-1.474019	4.479038	2.392061
H	-1.117412	2.106869	1.768071
H	-0.940340	1.292363	-3.019249
H	-0.401860	-0.358739	-2.648619
H	0.889341	2.233767	-1.559757
H	1.570119	1.216398	-2.829643

H	1.849263	-0.441499	4.623290
H	-0.503938	-2.421473	4.480669
H	-0.169797	-1.231307	5.727116
H	-0.416765	0.589432	3.875285
H	-1.836091	-0.186177	4.536468
H	-1.819779	-1.821733	2.501814
H	-2.313534	-0.142055	2.226506
P	-1.713392	0.183611	-0.736753
C	-2.962379	1.409619	-0.209177
C	-4.324714	1.294359	-0.523893
C	-5.226888	2.264422	-0.075689
C	-4.778126	3.349049	0.683010
C	-3.419285	3.468812	0.997018
C	-2.515016	2.501299	0.557921
H	-1.454909	2.600374	0.810683
H	-3.065054	4.314535	1.591277
H	-5.488129	4.101862	1.033809
H	-6.287160	2.169615	-0.322415
H	-4.685922	0.449497	-1.113668
C	-2.606967	-1.239847	-1.447047
C	-2.548189	-1.581392	-2.807040
C	-3.219066	-2.716603	-3.273807
C	-3.953184	-3.512622	-2.391204
C	-4.014288	-3.176620	-1.033676
C	-3.338872	-2.051580	-0.559744
H	-3.380036	-1.802817	0.503716
H	-4.585266	-3.797979	-0.339697
H	-4.477261	-4.397778	-2.759688
H	-3.168039	-2.975562	-4.334117
H	-1.983165	-0.973997	-3.516479
C	-0.783905	1.022248	-2.113026
C	0.597799	0.400421	-2.346958
P	1.578130	0.418573	-0.762271
C	1.925771	2.201112	-0.494926
C	1.514565	2.803087	0.706705
C	1.727711	4.167679	0.929238
C	2.356730	4.941150	-0.049266
C	2.777297	4.349219	-1.246848
C	2.565461	2.987640	-1.469788
H	2.907264	2.534012	-2.403781
H	3.275299	4.952984	-2.009367
H	2.525105	6.007236	0.121626
H	1.404933	4.623523	1.868352
H	1.031369	2.208983	1.488347
C	3.193474	-0.342870	-1.153454
C	4.331157	0.061183	-0.430758
C	5.556856	-0.576527	-0.632281
C	5.662065	-1.624615	-1.552846
C	4.535152	-2.032514	-2.272096
C	3.304726	-1.399642	-2.073559
H	2.437120	-1.741586	-2.641074
H	4.611177	-2.848840	-2.994529
H	6.622500	-2.121027	-1.710922
H	6.435137	-0.249732	-0.070085
H	4.264646	0.884168	0.285593
H	0.504014	-0.648240	-2.668548
H	1.145414	0.941305	-3.134489
H	-1.392446	1.029988	-3.030164
H	-0.688957	2.073343	-1.797225

^{4}10A-02
Geometry with 77 atoms:
Total energy: -3045.619216020

Cr	0.053807	-0.758215	0.899076
C	-0.350291	-2.480144	-0.116695
C	-1.719377	-3.128579	0.095745
C	-2.000558	-3.732150	1.484347
C	-2.587075	-2.777147	2.535330
C	-1.739224	-1.611894	3.062008
C	-0.531190	-1.940686	3.955735
C	0.761079	-2.404182	3.269088
C	1.371746	-1.349872	2.339210
H	2.349828	-1.677897	1.950166
H	1.554062	-0.398134	2.888118
H	0.586315	-3.340876	2.714519
H	1.484550	-2.669748	4.063817
H	-0.860684	-2.700836	4.684858
H	-0.289979	-1.040780	4.549255
H	-2.413826	-0.951655	3.632455
H	-1.472151	-0.933219	2.205144
H	-2.891592	-3.369345	3.416314

^{4}10A-03
Geometry with 77 atoms:
Total energy: -3045.620139010

Cr	-0.081752	-0.558651	0.968123
C	-1.451646	-0.779184	2.498241
C	-0.951888	-0.383571	3.901845
C	-0.080800	-1.415020	4.643538
C	1.420292	-1.411358	4.314738
C	1.795334	-1.669562	2.856437
C	1.420747	-3.046375	2.297316
C	1.410406	-3.104116	0.764283
C	0.189700	-2.415295	0.152949
H	-0.746325	-2.941739	0.408641
H	0.253431	-2.364133	-0.947701
H	1.427615	-4.162587	0.442378
H	2.342632	-2.659473	0.373046
H	0.431942	-3.357940	2.672187
H	2.144065	-3.773287	2.703038
H	2.876115	-1.504589	2.708142
H	1.380782	-0.817412	2.251785
H	1.923544	-2.174945	4.933660

^{4}10A-04
Geometry with 77 atoms:
Total energy: -3045.619715490

Cr	0.037184	-0.408486	1.084566
C	-0.350992	-2.362488	0.581388
C	-1.762941	-2.927411	0.761209
C	-2.218430	-3.257067	2.193423
C	-2.736256	-2.078057	3.030320
C	-1.731069	-0.957934	3.295398
C	-0.500803	-1.337214	4.125270
C	0.647537	-0.329916	4.001599
C	1.370815	-0.421439	2.646564
H	1.945902	-1.364212	2.585037
H	2.096268	0.404046	2.524708
H	1.365071	-0.492095	4.827894
H	0.250059	0.691652	4.159737
H	-0.132107	-2.333346	3.829427
H	-0.827530	-1.431014	5.174840
H	-2.235873	-0.097225	3.766174
H	-1.468221	-0.530820	2.290289
H	-3.088121	-2.456119	4.006341

H	-3.622917	-1.649621	2.530875
H	-1.400032	-3.774170	2.724211
H	-3.037978	-3.992083	2.131467
H	-2.510373	-2.269698	0.281010
H	-1.807949	-3.869929	0.182122
H	0.396301	-2.937884	1.156966
H	-0.053874	-2.413358	-0.480891
P	1.788696	0.051357	-0.632772
C	2.488876	-1.502091	-1.289762
C	2.450238	-1.848308	-2.649662
C	2.974053	-3.073452	-3.075659
C	3.541928	-3.955653	-2.153034
C	3.584780	-3.614551	-0.796265
C	3.054103	-2.399083	-0.364072
H	3.080452	-2.143421	0.697857
H	4.026712	-4.301488	-0.070662
H	3.951053	-4.911096	-2.490089
H	2.939944	-3.335235	-4.135933
H	2.019132	-1.172829	-3.390595
C	3.195792	1.125869	-0.172145
C	2.905561	2.340608	0.475591
C	3.937358	3.203172	0.847302
C	5.267880	2.856122	0.585911
C	5.560913	1.648132	-0.052541
C	4.530781	0.782288	-0.433794
H	4.772303	-0.158246	-0.932765
H	6.598670	1.374627	-0.258093
H	6.076558	3.528054	0.883314
H	3.703371	4.145739	1.348122
H	1.869767	2.618505	0.690556
C	0.985420	0.943596	-2.055378
C	-0.431916	0.435170	-2.344326
P	-1.469671	0.531152	-0.802183
C	-3.140298	-0.045860	-1.260749
C	-3.379872	-0.859606	-2.379986
C	-4.663446	-1.360471	-2.621499
C	-5.714795	-1.055740	-1.753467
C	-5.482425	-0.243609	-0.637219
C	-4.203637	0.255818	-0.388921
H	-4.032553	0.887574	0.487350
H	-6.301503	0.001502	0.043222
H	-6.715776	-1.449209	-1.945627
H	-4.840370	-1.990625	-3.496500
H	-2.575638	-1.112045	-3.073703
C	-1.622892	2.331315	-0.497428
C	-1.028683	2.847820	0.666373
C	-1.066465	4.218757	0.938024
C	-1.707225	5.081254	0.043909
C	-2.310585	4.573892	-1.114157
C	-2.270113	3.205020	-1.386943
H	-2.750922	2.814136	-2.287907
H	-2.816209	5.250855	-1.807020
H	-1.742404	6.153520	0.251285
H	-0.601050	4.610368	1.845613
H	-0.533700	2.167130	1.370417
H	-0.900615	1.019748	-3.151731
H	-0.409247	-0.619040	-2.663069
H	0.965447	2.003372	-1.755975
H	1.631007	0.886726	-2.945176

^{4}10A-05
Geometry with 77 atoms:
Total energy: -3045.619976410

Cr	0.123616	-0.655099	0.999660
C	0.021556	-2.478146	0.062053
C	-1.269825	-3.301701	0.110677
C	-1.677998	-3.922356	1.460255
C	-2.517602	-3.024499	2.382208
C	-1.806838	-1.774940	2.900905
C	-0.658685	-2.031653	3.884643
C	0.384218	-0.911483	3.928049
C	1.283061	-0.898266	2.679011
H	1.854361	-1.839982	2.601234
H	2.013611	-0.068559	2.729300
H	1.004665	-1.026201	4.837113
H	-0.128523	0.063507	4.055077
H	-0.145286	-2.972851	3.627479
H	-1.103011	-2.188914	4.881644
H	-2.531784	-1.077885	3.354062
H	-1.486453	-1.198028	1.991942
H	-2.853084	-3.611399	3.255449
H	-3.433552	-2.724079	1.844431
H	-0.777609	-4.282433	1.987975
H	-2.278096	-4.823909	1.254843
H	-2.115388	-2.718451	-0.292867
H	-1.139179	-4.134257	-0.606925
H	0.872064	-3.033995	0.496639
H	0.277126	-2.262994	-0.992336
P	1.867641	0.192361	-0.530908
C	3.294589	-0.897451	-0.847326
C	4.022735	-1.353592	0.267054
C	5.125026	-2.190683	0.090417
C	5.504980	-2.589239	-1.196084
C	4.780884	-2.145493	-2.305741
C	3.679807	-1.300017	-2.136906
H	3.135197	-0.961251	-3.019594
H	5.073822	-2.454855	-3.311955
H	6.365470	-3.248591	-1.332856
H	5.686380	-2.537505	0.961258
H	3.726697	-1.055384	1.274912
C	2.537782	1.844835	-0.112450
C	1.702529	2.758498	0.555342
C	2.151601	4.051206	0.834437
C	3.442785	4.436976	0.460416
C	4.282626	3.528402	-0.192276
C	3.835534	2.236386	-0.481031
H	4.499655	1.532832	-0.988298
H	5.293944	3.826604	-0.479317
H	3.797309	5.446506	0.682106
H	1.492310	4.755029	1.347996
H	0.693454	2.468839	0.860091
C	1.022380	0.449039	-2.169967
C	-0.262061	1.277250	-2.026397
P	-1.423975	0.610900	-0.721356
C	-2.660434	-0.411165	-1.600952
C	-2.339196	-1.103539	-2.779922
C	-3.255398	-1.997575	-3.342871
C	-4.496254	-2.210253	-2.736376
C	-4.824181	-1.519528	-1.564381
C	-3.912494	-0.628010	-0.996483
H	-4.179468	-0.097403	-0.078587
H	-5.795305	-1.676354	-1.088455
H	-5.208741	-2.911923	-3.176483
H	-2.995053	-2.531487	-4.260052
H	-1.373030	-0.960730	-3.268480
C	-2.335821	2.083977	-0.130023
C	-3.160102	2.834278	-0.987371
C	-3.808602	3.975703	-0.513138
C	-3.643613	4.377857	0.818123
C	-2.831492	3.634455	1.678592
C	-2.181469	2.489720	1.206152
H	-1.555496	1.908605	1.889737
H	-2.706792	3.940965	2.719890
H	-4.155104	5.270999	1.185223
H	-4.449041	4.553840	-1.183722
H	-3.303002	2.520531	-2.024523
H	-0.020065	2.303706	-1.710116
H	-0.786428	1.356000	-2.991373
H	1.720485	0.945818	-2.861887
H	0.810998	-0.554849	-2.570274

^{4}10A-06
Geometry with 77 atoms:
Total energy: -3045.620063400

Cr	0.086204	-0.414327	1.064210
C	-0.203518	-2.344809	0.461713
C	-1.525476	-3.003413	0.856800
C	-1.792267	-3.214109	2.359566
C	-2.489140	-2.056504	3.092084
C	-1.757111	-0.719257	3.269273
C	-0.590820	-0.660047	4.270622
C	0.752972	-1.258742	3.833442
C	1.379873	-0.533262	2.637700
H	2.370400	-0.950404	2.391393
H	1.544312	0.542306	2.875907
H	0.638081	-2.331133	3.606207
H	1.437830	-1.218880	4.702392
H	-0.933795	-1.146401	5.200017
H	-0.418310	0.399451	4.533370
H	-2.507681	0.025923	3.581866
H	-1.485708	-0.309768	2.256248
H	-2.773111	-2.398069	4.103066
H	-3.439521	-1.853425	2.567449
H	-0.856989	-3.497177	2.869433
H	-2.457600	-4.086962	2.464396
H	-2.377362	-2.462720	0.407253
H	-1.543216	-4.000159	0.374814
H	0.661452	-2.876320	0.897016
H	-0.077280	-2.358126	-0.635488
P	-1.473677	0.536346	-0.776842
C	-1.891223	2.310414	-0.578395
C	-2.598472	3.015335	-1.568594
C	-2.869326	4.374436	-1.403581
C	-2.440254	5.042946	-0.249995
C	-1.743268	4.349517	0.742715
C	-1.471411	2.987026	0.579246
H	-0.936487	2.449525	1.368574
H	-1.414451	4.866782	1.647202
H	-2.655796	6.106830	-0.124402
H	-3.420678	4.915498	-2.176475
H	-2.948299	2.497930	-2.465985
C	-3.041741	-0.291746	-1.221420
C	-4.187643	-0.003427	-0.456757
C	-5.374058	-0.706872	-0.671072
C	-5.431210	-1.709180	-1.646013
C	-4.297196	-2.000793	-2.408349
C	-3.105818	-1.299429	-2.198447
H	-2.232125	-1.554771	-2.800828
H	-4.335801	-2.780644	-3.172860
H	-6.359965	-2.260294	-1.811806
H	-6.258631	-0.470310	-0.074657
H	-4.156369	0.777278	0.308120
C	-0.407111	0.509886	-2.305918
C	0.975208	1.089724	-1.985860
P	1.812884	0.168963	-0.602441
C	3.162878	1.280981	-0.069045
C	2.810888	2.438823	0.648648
C	3.796377	3.331923	1.070768
C	5.142376	3.071054	0.789957
C	5.497369	1.918968	0.083027
C	4.513687	1.023652	-0.348651
H	4.803123	0.127709	-0.901281
H	6.547613	1.713502	-0.137805
H	5.914968	3.767024	1.125507
H	3.514494	4.230571	1.624750
H	1.761939	2.650935	0.877160
C	2.584818	-1.319244	-1.328840
C	3.199969	-2.230360	-0.450014
C	3.790731	-3.394175	-0.942558
C	3.757626	-3.671751	-2.313806
C	3.137327	-2.777825	-3.190229
C	2.554091	-1.603275	-2.703664
H	2.083737	-0.917224	-3.410160
H	3.109001	-2.990467	-4.261604
H	4.214720	-4.586783	-2.698028
H	4.271953	-4.090824	-0.252109
H	3.217038	-2.028117	0.623034
H	1.628604	1.112805	-2.871371
H	0.891136	2.131166	-1.636258
H	-0.317033	-0.536020	-2.637308
H	-0.895955	1.075181	-3.114692

^{4}10A-07
Geometry with 77 atoms:
Total energy: -3045.620388620

Cr	-0.158243	-0.730733	0.907192
C	-1.517801	-1.117375	2.398639
C	-0.984050	-0.851035	3.820162
C	-0.127539	-1.962742	4.455074
C	1.362639	-1.984466	4.082492
C	1.692274	-2.137303	2.598393
C	1.228348	-3.431425	1.923368
C	1.190051	-3.328084	0.392843
C	0.016890	-2.490372	-0.123854
H	-0.949402	-2.994348	0.049801
H	0.119006	-2.288543	-1.203880
H	1.127729	-4.344713	-0.038752
H	2.144033	-2.907822	0.030393
H	0.230223	-3.720900	2.290303
H	1.915354	-4.235126	2.236955
H	2.777723	-2.018408	2.441749
H	1.316043	-1.218536	2.070121
H	1.852889	-2.812493	4.624042

H	1.837092	-1.058870	4.454417
H	-0.590125	-2.939113	4.229539
H	-0.180317	-1.858735	5.551516
H	-0.421276	0.106983	3.865902
H	-1.849937	-0.684227	4.487685
H	-1.868176	-2.160310	2.298808
H	-2.403571	-0.483656	2.208445
P	-1.772241	0.213295	-0.678379
C	-2.289142	1.913132	-0.238797
C	-2.881705	2.766819	-1.186901
C	-3.228702	4.072193	-0.834315
C	-2.991410	4.537247	0.464774
C	-2.412243	3.692579	1.415075
C	-2.063286	2.384654	1.065608
H	-1.628638	1.724451	1.820008
H	-2.233708	4.049101	2.432240
H	-3.263076	5.560335	0.735903
H	-3.688262	4.730107	-1.575817
H	-3.081583	2.414143	-2.201970
C	-3.284092	-0.737212	-1.055228
C	-4.544753	-0.304047	-0.610752
C	-5.679001	-1.082362	-0.858371
C	-5.566211	-2.294419	-1.545114
C	-4.311880	-2.733812	-1.982080
C	-3.173382	-1.964977	-1.734364
H	-2.199722	-2.330393	-2.067548
H	-4.217707	-3.682629	-2.515711
H	-6.455713	-2.898613	-1.739079
H	-6.656025	-0.736008	-0.512837
H	-4.647420	0.642489	-0.076042
C	-0.862747	0.406145	-2.290105
C	0.446838	1.181358	-2.091342
P	1.522119	0.483215	-0.729535
C	2.481875	1.926311	-0.139259
C	2.146579	2.490903	1.102891
C	2.818345	3.624510	1.569431
C	3.834104	4.198191	0.799788
C	4.178072	3.638118	-0.436356
C	3.507159	2.507643	-0.906592
H	3.788670	2.070298	-1.867759
H	4.974874	4.084491	-1.036280
H	4.363256	5.081882	1.164756
H	2.551154	4.056478	2.536861
H	1.356371	2.046750	1.715254
C	2.732450	-0.615848	-1.552033
C	3.935072	-0.919605	-0.887121
C	4.827495	-1.845356	-1.429846
C	4.527451	-2.488411	-2.636000
C	3.334637	-2.193244	-3.301046
C	2.440049	-1.261465	-2.764536
H	1.516783	-1.045391	-3.306086
H	3.096700	-2.688312	-4.245692
H	5.225025	-3.215965	-3.057613
H	5.761677	-2.066479	-0.907781
H	4.181366	-0.424777	0.055988
H	1.020328	1.239767	-3.029585
H	0.229118	2.216530	-1.784665
H	-0.684274	-0.610334	-2.673523
H	-1.511124	0.913381	-3.021114

[4]10A-08
Geometry with 77 atoms:
Total energy: -3045.620508780

Cr	-0.120691	-0.587582	0.970544
C	-1.336454	-0.768921	2.625354
C	-0.653665	-0.526410	3.984696
C	0.159215	-1.694446	4.573393
C	1.606681	-1.836106	4.078850
C	1.788681	-2.047918	2.578128
C	1.196607	-3.334906	1.997087
C	1.039951	-3.286099	0.472380
C	-0.125743	-2.403489	0.022829
H	-1.099192	-2.842797	0.303051
H	-0.117092	-2.258110	-1.071482
H	0.886334	-4.311988	0.088130
H	1.982629	-2.935135	0.017107
H	0.215509	-3.544408	2.453797
H	1.857943	-4.167213	2.290680
H	2.858501	-1.991747	2.315033
H	1.403967	-1.127364	2.060368
H	2.082860	-2.684875	4.600562
H	2.175037	-0.938502	4.380918
H	-0.395390	-2.634857	4.409057
H	0.206132	-1.568793	5.667780
H	-0.012315	0.379719	3.951601
H	-1.439565	-0.270572	4.720073
H	-1.848998	-1.747293	2.616688
H	-2.116947	0.001768	2.472194
P	-1.804528	0.264872	-0.631759
C	-2.433741	1.939713	-0.239484
C	-3.763767	2.318797	-0.483480
C	-4.187597	3.615320	-0.177995
C	-3.292900	4.540813	0.368109
C	-1.967641	4.168332	0.616642
C	-1.540605	2.872088	0.321030
H	-0.503265	2.595434	0.528947
H	-1.264894	4.885588	1.047429
H	-3.629912	5.552768	0.605490
H	-5.224684	3.902644	-0.367672
H	-4.471188	1.602554	-0.907206
C	-3.254405	-0.790020	-0.971494
C	-3.945156	-1.336846	0.125276
C	-5.061682	-2.148905	-0.081119
C	-5.495102	-2.429791	-1.381138
C	-4.812283	-1.890734	-2.474927
C	-3.696989	-1.071615	-2.275569
H	-3.187523	-0.656770	-3.146749
H	-5.148927	-2.104983	-3.492147
H	-6.366035	-3.069782	-1.541883
H	-5.591593	-2.568332	0.777362
H	-3.609950	-1.130012	1.142682
C	-0.922930	0.454706	-2.261011
C	0.430417	1.162957	-2.117480
P	1.520829	0.433622	-0.784278
C	2.573237	1.838953	-0.262469
C	3.496689	2.439007	-1.137088
C	4.243505	3.541460	-0.718215
C	4.078482	4.054233	0.574492
C	3.167249	3.460740	1.451868
C	2.418670	2.355268	1.034988
H	1.713239	1.894685	1.733208
H	3.041326	3.853782	2.463542
H	4.665943	4.916793	0.898490
H	4.959643	4.003052	-1.402367
H	3.637879	2.037834	-2.143942
C	2.646726	-0.737848	-1.625210
C	2.237417	-1.460791	-2.758227
C	3.071768	-2.437499	-3.310184
C	4.318223	-2.704714	-2.737619
C	4.731576	-1.989332	-1.608487
C	3.901151	-1.015257	-1.051162
H	4.236815	-0.462987	-0.169586
H	5.707128	-2.189588	-1.158679
H	4.968786	-3.467589	-3.171734
H	2.744434	-2.990537	-4.193907
H	1.267267	-1.273626	-3.222588
H	0.969591	1.169601	-3.077612
H	0.278982	2.214570	-1.828847
H	-0.805104	-0.565053	-2.659846
H	-1.568827	1.012218	-2.957022

[4]10A-09
Geometry with 77 atoms:
Total energy: -3045.618964910

Cr	0.100924	-0.519488	1.041896
C	-0.213465	-2.407745	0.274814
C	-1.566406	-2.982823	0.712500
C	-1.583070	-3.657176	2.095315
C	-0.805030	-2.914154	3.185785
C	-1.213499	-1.459675	3.433440
C	-0.283126	-0.702471	4.389401
C	1.188533	-0.707335	3.955760
C	1.430564	-0.155833	2.549220
H	2.497683	-0.208003	2.277956
H	1.167552	0.934371	2.510842
H	1.589070	-1.733610	4.013995
H	1.774100	-0.129331	4.695667
H	-0.374412	-1.149624	5.394182
H	-0.636397	0.340243	4.486105
H	-2.254459	-1.418916	3.797400
H	-1.313796	-0.880600	2.471458
H	0.266721	-2.954976	2.937511
H	-0.905580	-3.454851	4.142555
H	-1.147656	-4.667506	2.008139
H	-2.631484	-3.802563	2.409068
H	-2.338042	-2.192856	0.680252
H	-1.913497	-3.721837	-0.033425
H	0.643234	-3.028053	0.592779
H	-0.153133	-2.315620	-0.823151
P	1.688676	0.180519	-0.716964
C	2.517779	-1.263704	-1.467546
C	2.534982	-1.503566	-2.850639
C	3.170031	-2.642002	-3.356971
C	3.795901	-3.542416	-2.491045
C	3.782446	-3.308274	-1.111317
C	3.139393	-2.180700	-0.599298
H	3.116843	-2.012767	0.480542
H	4.267264	-4.011798	-0.430444
H	4.292562	-4.429894	-2.890554
H	3.176523	-2.822016	-4.434672
H	2.059228	-0.811541	-3.547655
C	2.991252	1.380099	-0.258029
C	4.357187	1.125764	-0.453633
C	5.307173	2.069918	-0.050866
C	4.903414	3.267799	0.544559
C	3.541698	3.526074	0.740106
C	2.588977	2.585731	0.346757
H	1.527929	2.797603	0.510035
H	3.221227	4.460990	1.206099
H	5.649510	4.001578	0.858778
H	6.369215	1.865826	-0.207315
H	4.685678	0.194678	-0.919487
C	0.724324	1.040789	-2.055168
C	-0.665830	0.430647	-2.264344
P	-1.622994	0.446735	-0.663932
C	-3.265402	-0.252362	-1.063040
C	-4.393684	0.194673	-0.351252
C	-5.639850	-0.399183	-0.561855
C	-5.774920	-1.444986	-1.480785
C	-4.657268	-1.895296	-2.189498
C	-3.406771	-1.307207	-1.981441
H	-2.546062	-1.683842	-2.537823
H	-4.756576	-2.710823	-2.910004
H	-6.751072	-1.907642	-1.644974
H	-6.510208	-0.040178	-0.007044
H	-4.303418	1.015764	0.364652
C	-1.915644	2.236897	-0.373910
C	-1.462628	2.822701	0.819910
C	-1.638429	4.190990	1.053517
C	-2.272429	4.984240	0.094431
C	-2.734841	4.408346	-1.095594
C	-2.559661	3.043590	-1.329797
H	-2.933909	2.602398	-2.257340
H	-3.237097	5.027179	-1.843076
H	-2.412490	6.052854	0.274844
H	-1.283294	4.633487	1.987339
H	-0.975720	2.214710	1.587651
H	-1.223849	0.983932	-3.035643
H	-0.588948	-0.615076	-2.600609
H	0.641378	2.088481	-1.725579
H	1.307762	1.060632	-2.988030

[4]10A-10
Geometry with 77 atoms:
Total energy: -3045.620338630

Cr	-0.077453	-0.534633	1.023561
C	-1.285697	-0.633506	2.659071
C	-0.344112	0.368820	3.315138
C	0.660726	-0.195895	4.340693
C	1.322041	-1.522342	3.936835
C	2.104087	-1.493084	2.614234
C	2.190151	-2.827144	1.862042
C	0.835508	-3.352562	1.363578
C	0.127899	-2.461378	0.332217
H	-0.870156	-2.863362	0.100238
H	0.704302	-2.432818	-0.611211
H	0.164720	-3.525027	2.222443
H	0.997321	-4.354484	0.921570
H	2.656783	-3.574952	2.526539
H	2.871123	-2.704417	1.002715
H	3.114828	-1.086799	2.786314
H	1.705485	-0.718937	1.909378
H	0.546839	-2.301311	3.889084

H	2.006401	-1.841213	4.739696
H	0.122649	-0.353692	5.290043
H	1.432511	0.566881	4.544471
H	0.268330	0.903064	2.509359
H	-0.881559	1.226103	3.753562
H	-1.342740	-1.611748	3.156007
H	-2.296911	-0.232657	2.498227
P	-1.794377	0.096394	-0.605762
C	-3.004545	1.355096	-0.058551
C	-2.513991	2.458748	0.663253
C	-3.384863	3.456541	1.102636
C	-4.754538	3.356829	0.832786
C	-5.247055	2.261173	0.118287
C	-4.378254	1.260836	-0.329232
H	-4.774414	0.409153	-0.885671
H	-6.315753	2.182089	-0.095413
H	-5.438238	4.134390	1.181842
H	-2.995557	4.311277	1.661026
H	-1.445684	2.544743	0.880910
C	-2.744682	-1.328348	-1.235999
C	-2.713716	-1.735266	-2.578397
C	-3.422314	-2.871877	-2.982691
C	-4.166087	-3.604460	-2.054812
C	-4.197337	-3.204645	-0.713380
C	-3.483762	-2.079105	-0.302034
H	-3.495034	-1.785152	0.750626
H	-4.773421	-3.777479	0.017173
H	-4.719604	-4.490727	-2.374324
H	-3.392267	-3.182418	-4.029800
H	-2.140997	-1.178505	-3.322430
C	-0.924948	0.886504	-2.051325
C	0.450889	0.257374	-2.309673
P	1.498358	0.426829	-0.777465
C	1.945238	2.203978	-0.766653
C	2.709316	2.769447	-1.803571
C	2.999359	4.134532	-1.796937
C	2.531983	4.948460	-0.757301
C	1.778370	4.393814	0.280034
C	1.488313	3.025303	0.276341
H	0.908582	2.596172	1.097992
H	1.418567	5.024373	1.096578
H	2.761400	6.016841	-0.755534
H	3.594748	4.566860	-2.604791
H	3.086609	2.139273	-2.613136
C	3.060008	-0.473920	-1.078433
C	4.182891	-0.129438	-0.302324
C	5.362446	-0.868790	-0.401561
C	5.435896	-1.962322	-1.271864
C	4.325644	-2.308858	-2.046161
C	3.140954	-1.571597	-1.951475
H	2.287023	-1.865403	-2.564194
H	4.378276	-3.158220	-2.731577
H	6.359545	-2.540967	-1.347843
H	6.229139	-0.588953	0.202301
H	4.139345	0.724075	0.379997
H	0.349814	-0.814511	-2.538759
H	0.952507	0.738269	-3.164007
H	-1.567914	0.855686	-2.944220
H	-0.822351	1.949828	-1.780867

H	1.879124	-0.700494	4.447201
H	-0.354039	-2.811076	4.312294
H	-0.089663	-1.582364	5.537954
H	-0.468377	0.186118	3.644858
H	-1.825805	-0.655343	4.345872
H	-1.621690	-2.377469	2.319869
H	-2.383135	-0.794433	2.070395
P	-1.730741	0.178396	-0.733291
C	-2.728922	1.474722	0.096137
C	-2.087997	2.640089	0.557502
C	-2.805101	3.601886	1.271483
C	-4.163965	3.407496	1.541787
C	-4.802285	2.247245	1.094838
C	-4.091063	1.280885	0.376991
H	-4.602692	0.379624	0.033425
H	-5.863529	2.090705	1.302811
H	-4.724282	4.160853	2.100698
H	-2.298655	4.506392	1.617322
H	-1.026236	2.811280	0.360942
C	-2.925721	-0.958451	-1.517721
C	-3.606314	-0.604985	-2.696359
C	-4.555359	-1.470444	-3.243449
C	-4.840010	-2.688533	-2.615956
C	-4.177386	-3.038526	-1.436325
C	-3.222640	-2.178268	-0.886728
H	-2.717299	-2.452725	0.040070
H	-4.402209	-3.985039	-0.939155
H	-5.583613	-3.363619	-3.046524
H	-5.079758	-1.189855	-4.160073
H	-3.412352	0.351584	-3.186721
C	-0.812679	1.065278	-2.099932
C	0.568930	0.455693	-2.361668
P	1.576152	0.417903	-0.797231
C	1.962434	2.176529	-0.454067
C	1.714269	2.685822	0.831741
C	1.987320	4.025149	1.129971
C	2.510481	4.864410	0.143122
C	2.768738	4.363259	-1.138993
C	2.500404	3.026366	-1.437164
H	2.719953	2.641019	-2.436239
H	3.186102	5.017929	-1.907932
H	2.723916	5.911265	0.372613
H	1.793210	4.410036	2.133970
H	1.310060	2.035164	1.612899
C	3.174071	-0.352162	-1.248469
C	3.266976	-1.334662	-2.249337
C	4.481866	-1.984394	-2.486605
C	5.611707	-1.666776	-1.727971
C	5.525783	-0.690033	-0.729966
C	4.315678	-0.036416	-0.489054
H	4.263796	0.728151	0.290642
H	6.406993	-0.432280	-0.137279
H	6.559330	-2.177340	-1.915647
H	4.542554	-2.743621	-3.270233
H	2.398133	-1.608214	-2.850433
H	0.465304	-0.584040	-2.708159
H	1.100837	1.012592	-3.148788
H	-1.419556	1.057964	-3.016975
H	-0.720276	2.117759	-1.792204

H	2.214652	-0.326930	4.411809
H	-0.519360	-1.687564	4.800993
H	0.213855	-0.434043	5.787913
H	0.175905	1.060672	3.620829
H	-1.268372	0.821632	4.571384
H	-1.945348	-1.106123	2.920465
H	-2.082439	0.577942	2.371938
P	1.546639	0.178520	-0.870250
C	2.687919	-1.006891	-1.678120
C	4.075128	-0.794232	-1.732027
C	4.905205	-1.739036	-2.343516
C	4.362360	-2.897543	-2.905892
C	2.981547	-3.117079	-2.849953
C	2.148268	-2.182795	-2.231833
H	1.074550	-2.376967	-2.179867
H	2.551438	-4.023537	-3.282774
H	5.014592	-3.631701	-3.384917
H	5.983102	-1.563325	-2.382557
H	4.513104	0.109383	-1.303051
C	2.580408	1.603454	-0.362502
C	3.042734	1.640106	0.965612
C	3.828604	2.704411	1.415313
C	4.155831	3.747057	0.543325
C	3.704340	3.717660	-0.780639
C	2.924492	2.651095	-1.235146
H	2.590845	2.640051	-2.275099
H	3.963838	4.528712	-1.465335
H	4.764587	4.583522	0.895115
H	4.181872	2.720268	2.449093
H	2.795689	0.827898	1.654740
C	0.465171	0.831009	-2.254790
C	-0.892309	0.119013	-2.323393
P	-1.787146	0.175811	-0.691590
C	-3.298582	-0.822715	-0.897657
C	-4.021736	-1.171894	0.257884
C	-5.188534	-1.930689	0.152751
C	-5.639894	-2.355448	-1.101640
C	-4.923397	-2.015461	-2.252250
C	-3.757394	-1.250124	-2.155335
H	-3.220586	-0.990592	-3.069296
H	-5.273069	-2.344116	-3.233946
H	-6.550832	-2.953510	-1.181834
H	-5.744445	-2.196007	1.055150
H	-3.673257	-0.851848	1.241707
C	-2.311294	1.921411	-0.509349
C	-3.585000	2.368188	-0.896211
C	-3.928219	3.714395	-0.742518
C	-3.007958	4.620956	-0.206324
C	-1.738405	4.181543	0.183640
C	-1.393210	2.836270	0.039151
H	-0.402221	2.501392	0.360950
H	-1.018485	4.884509	0.609436
H	-3.282909	5.671562	-0.085399
H	-4.922334	4.055886	-1.041210
H	-4.311495	1.665510	-1.310915
H	-1.522474	0.582861	-3.098262
H	-0.773181	-0.945449	-2.583238
H	0.316572	1.904642	-2.060915
H	0.994377	0.740764	-3.215311

^{4}10A-11
Geometry with 77 atoms:
Total energy: -3045.619030440

Cr	-0.078411	-0.781439	0.847772
C	-1.427632	-1.290278	2.318733
C	-0.940745	-0.819247	3.703965
C	0.003747	-1.776966	4.456681
C	1.500230	-1.684595	4.118107
C	1.884589	-1.882858	2.652635
C	1.555121	-3.243891	2.027934
C	1.563505	-3.217776	0.492397
C	0.319763	-2.548248	-0.101158
H	-0.578754	-3.162893	0.074272
H	0.412919	-2.398319	-1.191038
H	1.630967	-4.254616	0.112683
H	2.479726	-2.712436	0.141058
H	0.572477	-3.601361	2.376630
H	2.296138	-3.969155	2.403300
H	2.961070	-1.681775	2.518036
H	1.456603	-1.020628	2.071971
H	2.046639	-2.433228	4.718306

^{4}10A-12
Geometry with 77 atoms:
Total energy: -3045.618738480

Cr	-0.180594	-0.506957	1.027018
C	-1.359824	-0.202739	2.676082
C	-0.567101	0.285144	3.905489
C	0.132676	-0.798130	4.750556
C	1.547689	-1.201300	4.307959
C	1.674761	-1.747570	2.887775
C	0.960319	-3.072649	2.604562
C	0.723741	-3.324915	1.109837
C	-0.414504	-2.475444	0.539064
H	-1.387100	-2.755302	0.980226
H	-0.499974	-2.590257	-0.555618
H	0.491537	-4.395478	0.954392
H	1.659601	-3.140188	0.550828
H	-0.007882	-3.104901	3.131066
H	1.572938	-3.880005	3.039081
H	2.737955	-1.843690	2.609535
H	1.353951	-0.930249	2.188912
H	1.939673	-1.963794	5.003712

^{4}10A-13
Geometry with 77 atoms:
Total energy: -3045.618066950

Cr	-0.112647	-0.189083	1.207681
C	-0.091281	1.763130	1.810406
C	1.263059	2.383180	2.165708
C	1.845611	2.045386	3.549821
C	2.593779	0.708627	3.664171
C	1.775998	-0.546843	3.365005
C	0.598441	-0.831516	4.302428
C	-0.430991	-1.791870	3.697740
C	-1.288623	-1.127137	2.606099
H	-1.950141	-0.365933	3.057616
H	-1.941056	-1.867148	2.107491
H	-1.081780	-2.182729	4.502379
H	0.094601	-2.678833	3.293690
H	0.090070	0.108039	4.574724
H	1.011231	-1.239613	5.240439
H	2.436891	-1.429709	3.334257
H	1.469233	-0.484469	2.287499
H	3.002476	0.611396	4.685189

H	3.468920	0.732789	2.990086
H	1.042565	2.099775	4.305142
H	2.560697	2.838315	3.824280
H	2.014181	2.156227	1.386225
H	1.143642	3.482649	2.119187
H	-0.801341	1.822457	2.653267
H	-0.558404	2.285634	0.955933
P	1.471638	-0.074894	-0.917389
C	2.797717	-1.334718	-0.917055
C	2.958658	-2.300920	-1.924201
C	3.993245	-3.238468	-1.838800
C	4.878181	-3.215464	-0.757198
C	4.728278	-2.251965	0.246732
C	3.690870	-1.321301	0.171566
H	3.580750	-0.572161	0.961170
H	5.419894	-2.227561	1.092386
H	5.686891	-3.947825	-0.696567
H	4.110273	-3.986474	-2.626834
H	2.288827	-2.328567	-2.785908
C	2.251782	1.468245	-1.537587
C	3.478351	1.460505	-2.223460
C	4.015483	2.654535	-2.712081
C	3.336318	3.862916	-2.525684
C	2.116607	3.877784	-1.842235
C	1.579814	2.688567	-1.343009
H	0.640526	2.717155	-0.788001
H	1.585488	4.819732	-1.684946
H	3.761167	4.794183	-2.908054
H	4.970885	2.639436	-3.242337
H	4.018718	0.523719	-2.376767
C	0.308524	-0.549578	-2.298615
C	-0.998747	0.248545	-2.200786
P	-1.857577	-0.077007	-0.577544
C	-2.746659	-1.654643	-0.859588
C	-4.069595	-1.681943	-1.330418
C	-4.699490	-2.905084	-1.575360
C	-4.017562	-4.106230	-1.355931
C	-2.701580	-4.085993	-0.883354
C	-2.070130	-2.866183	-0.629592
H	-1.048014	-2.867243	-0.239253
H	-2.168164	-5.021975	-0.700971
H	-4.515196	-5.060210	-1.546407
H	-5.730359	-2.918636	-1.937299
H	-4.612714	-0.749735	-1.501968
C	-3.126794	1.217466	-0.388525
C	-3.524770	2.053722	-1.445248
C	-4.507430	3.025904	-1.233916
C	-5.099427	3.166749	0.024509
C	-4.708310	2.333941	1.078723
C	-3.724076	1.365545	0.876576
H	-3.417721	0.721916	1.704317
H	-5.167720	2.442284	2.064078
H	-5.867009	3.927783	0.184915
H	-4.813023	3.673393	-2.059302
H	-3.082638	1.954511	-2.438460
H	-0.803776	1.331083	-2.265705
H	-1.677945	-0.015896	-3.025971
H	0.792195	-0.380684	-3.272935
H	0.107980	-1.629924	-2.207985

H	-3.324724	-2.593315	2.134139
H	-0.557342	-3.898316	2.448452
H	-2.028172	-4.645676	1.856400
H	-2.040533	-2.742028	0.020487
H	-1.056138	-4.176958	-0.146536
H	0.983578	-2.919695	0.692704
H	0.303254	-2.321982	-0.841897
P	1.872858	0.234288	-0.529071
C	3.284181	-0.869086	-0.886439
C	3.975802	-0.802649	-2.110818
C	5.050148	-1.660114	-2.357579
C	5.446386	-2.588106	-1.388869
C	4.764868	-2.658188	-0.170686
C	3.687146	-1.805422	0.080929
H	3.153897	-1.875268	1.029429
H	5.068595	-3.383340	0.587872
H	6.286547	-3.258411	-1.586039
H	5.580839	-1.601316	-3.310902
H	3.688867	-0.080959	-2.878161
C	2.546956	1.879648	-0.084323
C	3.913310	2.188626	-0.180418
C	4.370565	3.460577	0.177426
C	3.474376	4.431844	0.632853
C	2.112695	4.129085	0.737163
C	1.651310	2.858655	0.387616
H	0.584507	2.640051	0.483919
H	1.406553	4.880932	1.097793
H	3.837380	5.423974	0.911857
H	5.435916	3.691121	0.100626
H	4.625766	1.439749	-0.531581
C	1.040430	0.475581	-2.183809
C	-0.292119	1.228889	-2.086310
P	-1.445665	0.526296	-0.793566
C	-2.598363	-0.589419	-1.672447
C	-3.842176	-0.879371	-1.080823
C	-4.696191	-1.818573	-1.660692
C	-4.316739	-2.487064	-2.830164
C	-3.082264	-2.205816	-3.421048
C	-2.224487	-1.261812	-2.847238
H	-1.264618	-1.059835	-3.327380
H	-2.782245	-2.722190	-4.336122
H	-4.984926	-3.224692	-3.280832
H	-5.662487	-2.030156	-1.196373
H	-4.148914	-0.365882	-0.165701
C	-2.456473	1.963094	-0.272527
C	-2.281474	2.480788	1.021927
C	-2.997943	3.607831	1.437130
C	-3.898028	4.221015	0.561648
C	-4.083522	3.706711	-0.727602
C	-3.368234	2.583024	-1.145369
H	-3.525290	2.180554	-2.149357
H	-4.791340	4.183528	-1.409975
H	-4.461286	5.099919	0.884689
H	-2.856644	4.001892	2.446380
H	-1.585730	2.003833	1.718580
H	-0.119620	2.275359	-1.792265
H	-0.797745	1.255288	-3.064230
H	1.725993	1.010655	-2.858699
H	0.903284	-0.539843	-2.589586

H	2.325674	-1.477523	4.440268
H	0.135403	-1.118442	5.450719
H	0.378634	-0.073588	4.062004
H	-1.935998	-1.358212	4.496583
H	-1.152476	-2.689994	3.674727
H	-2.471492	-1.400347	2.032684
H	-1.757834	0.130221	2.581534
P	-1.785178	0.264695	-0.671187
C	-2.244183	1.989478	-0.262992
C	-1.370786	2.744150	0.540560
C	-1.649059	4.083600	0.822994
C	-2.808748	4.676358	0.314709
C	-3.685266	3.929969	-0.480806
C	-3.406226	2.592927	-0.773603
H	-4.097711	2.018448	-1.394330
H	-4.592488	4.392205	-0.877392
H	-3.031946	5.722059	0.539921
H	-0.960052	4.661185	1.443740
H	-0.458859	2.294289	0.941966
C	-3.331012	-0.648921	-0.972500
C	-4.340383	-0.587224	0.007464
C	-5.508174	-1.336488	-0.140023
C	-5.678951	-2.159169	-1.259117
C	-4.678749	-2.227636	-2.232424
C	-3.506567	-1.478097	-2.092958
H	-2.740426	-1.547670	-2.866982
H	-4.808933	-2.866801	-3.108905
H	-6.593450	-2.746355	-1.371941
H	-6.287577	-1.279152	0.623598
H	-4.216669	0.053339	0.883693
C	-0.884663	0.400795	-2.293963
C	0.463873	1.116374	-2.120545
P	1.517049	0.400404	-0.745513
C	2.490840	1.826954	-0.141081
C	2.443711	2.157216	1.223135
C	3.149062	3.262942	1.709311
C	3.905926	4.044773	0.832886
C	3.962670	3.718839	-0.528008
C	3.261851	2.614356	-1.014842
H	3.318250	2.361650	-2.076832
H	4.558863	4.328035	-1.211722
H	4.457326	4.909718	1.209656
H	3.107897	3.510779	2.772654
H	1.856724	1.548030	1.916739
C	2.726038	-0.709488	-1.556734
C	3.982557	-0.914556	-0.958630
C	4.871688	-1.850619	-1.490936
C	4.516673	-2.596703	-2.619798
C	3.269205	-2.398444	-3.218277
C	2.375547	-1.462072	-2.690416
H	1.404954	-1.329828	-3.172847
H	2.987422	-2.975212	-4.102594
H	5.213368	-3.329278	-3.034115
H	5.848141	-1.995810	-1.022257
H	4.273585	-0.335819	-0.078083
H	1.029352	1.111509	-3.064913
H	0.300417	2.170363	-1.846614
H	-0.744328	-0.623037	-2.672138
H	-1.520619	0.937971	-3.015435

[4]10A-14
Geometry with 77 atoms:
Total energy: -3045.619330490

Cr	0.112009	-0.541234	1.012787
C	0.103315	-2.430518	0.240137
C	-1.165863	-3.255848	0.457520
C	-1.490604	-3.684152	1.902011
C	-2.389268	-2.730915	2.705101
C	-1.865618	-1.341410	3.091393
C	-0.786329	-1.254405	4.182473
C	0.659332	-1.568826	3.776193
C	1.217440	-0.610134	2.718882
H	2.300026	-0.756699	2.576112
H	1.089095	0.449541	3.045943
H	0.742508	-2.609690	3.422103
H	1.281930	-1.523814	4.690346
H	-1.095806	-1.917193	5.008980
H	-0.801640	-0.230801	4.598080
H	-2.731567	-0.742535	3.419309
H	-1.568032	-0.784718	2.160793
H	-2.685214	-3.231478	3.643854

[4]10A-15
Geometry with 77 atoms:
Total energy: -3045.617447950

Cr	-0.189126	-0.749306	0.888295
C	-1.540286	-0.951275	2.419049
C	-1.145116	-1.589726	3.758709
C	0.204718	-1.129783	4.350518
C	1.446528	-1.960566	3.982871
C	1.702646	-2.163062	2.482356
C	1.107409	-3.437067	1.865299
C	1.006590	-3.385020	0.336134
C	-0.152195	-2.509274	-0.144446
H	-1.130303	-2.963345	0.094634
H	-0.106899	-2.336875	-1.233254
H	0.877526	-4.411268	-0.055834
H	1.961020	-3.021935	-0.084589
H	0.109867	-3.636340	2.288578
H	1.745336	-4.278946	2.182049
H	2.783056	-2.146222	2.263196
H	1.382371	-1.225664	1.946547
H	1.370821	-2.956544	4.453350

[4]10A-16
Geometry with 77 atoms:
Total energy: -3045.620307740

Cr	-0.071036	-0.794104	0.834349
C	-1.444396	-1.116560	2.312832
C	-0.553140	-0.314728	3.254954
C	0.296716	-1.131050	4.250990
C	0.932924	-2.401783	3.669701
C	1.874723	-2.184460	2.476179
C	1.991014	-3.368054	1.508174
C	0.701915	-3.671163	0.729829
C	0.247640	-2.544980	-0.210964
H	-0.670580	-2.834261	-0.745616
H	1.028821	-2.361822	-0.971163
H	-0.110288	-3.927942	1.431631
H	0.867596	-4.590212	0.135553
H	2.298539	-4.260047	2.081141
H	2.803688	-3.162864	0.790280
H	2.873283	-1.888608	2.839510
H	1.604660	-1.271186	1.884319
H	0.131467	-3.098973	3.383006

H	1.495663	-2.917593	4.464702
H	-0.354867	-1.426442	5.090078
H	1.076575	-0.477966	4.680097
H	0.162486	0.334262	2.649964
H	-1.116190	0.463947	3.795870
H	-1.594398	-2.164435	2.607986
H	-2.421240	-0.641684	2.142891
P	-1.714410	0.166770	-0.697173
C	-2.669945	1.496996	0.130154
C	-4.029095	1.335264	0.445103
C	-4.703020	2.324344	1.167950
C	-4.030873	3.476549	1.585648
C	-2.675843	3.640388	1.278737
C	-1.996264	2.655380	0.559572
H	-0.937002	2.801255	0.335247
H	-2.142856	4.538945	1.599473
H	-4.562141	4.247512	2.148940
H	-5.761943	2.192080	1.402951
H	-4.567847	0.441009	0.125533
C	-2.958553	-0.957782	-1.423653
C	-3.633726	-0.637564	-2.614226
C	-4.626752	-1.486783	-3.107261
C	-4.961109	-2.654640	-2.413140
C	-4.302473	-2.971579	-1.221694
C	-3.303803	-2.128674	-0.726793
H	-2.794682	-2.378639	0.205486
H	-4.563948	-3.879960	-0.673772
H	-5.738969	-3.316793	-2.801161
H	-5.146128	-1.231893	-4.034183
H	-3.401486	0.281207	-3.157569
C	-0.798428	1.005065	-2.096114
C	0.593396	0.396674	-2.314602
P	1.572212	0.430485	-0.733759
C	1.972230	2.201930	-0.475516
C	2.573157	2.973650	-1.486314
C	2.855856	4.322457	-1.265941
C	2.549257	4.913741	-0.033984
C	1.964192	4.151954	0.980451
C	1.677323	2.800327	0.760641
H	1.221461	2.211214	1.561061
H	1.731371	4.607450	1.945962
H	2.773325	5.969851	0.134997
H	3.321849	4.915488	-2.056631
H	2.830807	2.518957	-2.446419
C	3.174934	-0.370959	-1.102481
C	3.401924	-1.140282	-2.255180
C	4.623417	-1.800292	-2.428506
C	5.624008	-1.698844	-1.459074
C	5.405039	-0.929896	-0.309854
C	4.187620	-0.272537	-0.129955
H	4.025803	0.327620	0.770191
H	6.186293	-0.843022	0.449224
H	6.576360	-2.215902	-1.598867
H	4.791772	-2.394627	-3.329874
H	2.637487	-1.232908	-3.028584
H	0.505616	-0.658088	-2.618865
H	1.130302	0.929313	-3.115148
H	-1.393679	0.951730	-3.018948
H	-0.718314	2.071054	-1.833649

^{4}10A-17
Geometry with 77 atoms:
Total energy: -3045.617888650

Cr	-0.164801	-0.834010	0.844201
C	-1.429988	-1.289739	2.366825
C	-1.027840	-2.314151	3.431818
C	0.381797	-2.178489	4.046142
C	1.517773	-2.937216	3.336773
C	2.019780	-2.384322	1.982844
C	1.925949	-3.346596	0.791651
C	0.496884	-3.670833	0.338907
C	-0.218434	-2.496497	-0.333940
H	-1.275927	-2.732632	-0.539005
H	0.279948	-2.233949	-1.285215
H	-0.095225	-4.034440	1.195900
H	0.537128	-4.520969	-0.368559
H	2.447416	-4.275678	1.079356
H	2.489380	-2.929948	-0.059864
H	3.062326	-2.041607	2.080869
H	1.515352	-1.405049	1.754564
H	1.197733	-3.984177	3.200281
H	2.377263	-2.980492	4.024906
H	0.342561	-2.558671	5.080037
H	0.648277	-1.107068	4.141146
H	-1.759664	-2.255011	4.259896
H	-1.142993	-3.334773	3.025837
H	-2.433555	-1.522201	1.971876
H	-1.494980	-0.272097	2.823297
P	-1.806593	0.315698	-0.573207
C	-2.282027	2.010917	-0.072174
C	-1.440113	2.722165	0.800163
C	-1.732542	4.044286	1.144065
C	-2.874661	4.662233	0.626666
C	-3.720655	3.958306	-0.238149
C	-3.427844	2.639097	-0.590753
H	-4.095664	2.096759	-1.264214
H	-4.614361	4.440271	-0.641873
H	-3.108345	5.694582	0.898106
H	-1.067108	4.588571	1.818319
H	-0.540799	2.252172	1.205929
C	-3.352383	-0.583286	-0.920111
C	-4.367947	-0.565386	0.054616
C	-5.537391	-1.302417	-0.136898
C	-5.703368	-2.069149	-1.295717
C	-4.695621	-2.095955	-2.263226
C	-3.521777	-1.358800	-2.079177
H	-2.748834	-1.396922	-2.848376
H	-4.821218	-2.692110	-3.170214
H	-6.619545	-2.645722	-1.444019
H	-6.322199	-1.278754	0.622937
H	-4.248540	0.032107	0.961707
C	-0.923954	0.548738	-2.195882
C	0.394472	1.311851	-1.997570
P	1.473476	0.560650	-0.664432
C	2.375388	1.980409	0.057515
C	2.300129	2.206305	1.442092
C	2.954199	3.300320	2.018102
C	3.687837	4.175168	1.212663
C	3.773482	3.953271	-0.167395
C	3.124073	2.860570	-0.744145
H	3.205219	2.689643	-1.820881
H	4.352254	4.634326	-0.796045
H	4.199101	5.030863	1.660441
H	2.891065	3.467108	3.096091
H	1.730882	1.525558	2.082115
C	2.745051	-0.425739	-1.537624
C	3.998387	-0.623085	-0.930352
C	4.936152	-1.478570	-1.512218
C	4.633963	-2.150641	-2.701495
C	3.390932	-1.957807	-3.311028
C	2.448438	-1.101466	-2.733599
H	1.483520	-0.966305	-3.227597
H	3.150821	-2.476108	-4.242571
H	5.368168	-2.821442	-3.153857
H	5.908833	-1.619430	-1.034498
H	4.248041	-0.102611	-0.002201
H	0.954042	1.374804	-2.943336
H	0.192365	2.344006	-1.671949
H	-0.744055	-0.457073	-2.606815
H	-1.585545	1.084529	-2.895070

^{4}10A-18
Geometry with 77 atoms:
Total energy: -3045.617541840

Cr	0.168682	-0.553528	1.024825
C	0.155880	-2.438741	0.210380
C	-1.101588	-3.203173	0.639660
C	-1.028646	-3.913341	2.002579
C	-0.470254	-3.071856	3.156685
C	-1.187290	-1.737860	3.409088
C	-0.435207	-0.774835	4.348142
C	0.461889	0.238829	3.620212
C	1.460121	-0.350162	2.613175
H	1.940412	-1.270906	2.978911
H	2.252188	0.381140	2.379826
H	0.984576	0.867218	4.365154
H	-0.205514	0.973267	3.103987
H	0.180636	-1.367946	5.045866
H	-1.154708	-0.220000	4.971737
H	-2.203092	-1.943175	3.786800
H	-1.411797	-1.210378	2.445437
H	0.598458	-2.884228	2.975001
H	-0.510518	-3.658838	4.089888
H	-0.394245	-4.811097	1.904459
H	-2.038054	-4.279604	2.260846
H	-1.974553	-2.524824	0.621724
H	-1.346748	-3.960574	-0.127858
H	1.091638	-2.944339	0.505741
H	0.173217	-2.307365	-0.885755
P	1.771600	0.258408	-0.631712
C	3.248359	-0.759269	-0.967710
C	3.819742	-0.841214	-2.250336
C	4.954864	-1.627785	-2.462894
C	5.530623	-2.333287	-1.401719
C	4.968305	-2.253402	-0.123964
C	3.830499	-1.473594	0.094276
H	3.392650	-1.423123	1.091941
H	5.413481	-2.804969	0.707453
H	6.418054	-2.947671	-1.572044
H	5.391135	-1.687727	-3.462881
H	3.391547	-0.291637	-3.090809
C	2.339730	1.966689	-0.291942
C	1.411340	2.881408	0.240256
C	1.788912	4.200303	0.499548
C	3.100535	4.614092	0.243660
C	4.031054	3.706214	-0.270918
C	3.656468	2.386324	-0.539675
H	4.392325	1.684470	-0.938042
H	5.058128	4.025297	-0.464199
H	3.398928	5.644516	0.451395
H	1.058581	4.903109	0.907729
H	0.385536	2.570580	0.455772
C	0.858322	0.372875	-2.251731
C	-0.506204	1.059655	-2.105703
P	-1.564256	0.375654	-0.720246
C	-2.678819	-0.851406	-1.499914
C	-2.274793	-1.612432	-2.609406
C	-3.100150	-2.625706	-3.107036
C	-4.332074	-2.891060	-2.503283
C	-4.740910	-2.135912	-1.398607
C	-3.919718	-1.125342	-0.895896
H	-4.250960	-0.543585	-0.031623
H	-5.705394	-2.334403	-0.924765
H	-4.974869	-3.683412	-2.894036
H	-2.776789	-3.208701	-3.972821
H	-1.316813	-1.427072	-3.099042
C	-2.645497	1.785306	-0.269483
C	-2.543372	2.347062	1.013836
C	-3.324737	3.452050	1.367816
C	-4.216244	3.999928	0.442231
C	-4.329264	3.441426	-0.837009
C	-3.550178	2.339650	-1.193387
H	-3.653558	1.903888	-2.190339
H	-5.030654	3.865942	-1.559443
H	-4.829076	4.861742	0.717617
H	-3.238994	3.879807	2.369557
H	-1.857141	1.921262	1.750916
H	-0.368257	2.125694	-1.868359
H	-1.065721	1.015717	-3.052940
H	1.474897	0.920276	-2.981303
H	0.762365	-0.663197	-2.613537

^{4}10A-19
Geometry with 77 atoms:
Total energy: -3045.617589730

Cr	-0.092199	-0.647521	0.950145
C	-1.408084	-1.182707	2.435585
C	-0.829251	-1.221110	3.860485
C	0.189941	-2.336171	4.169586
C	1.669055	-2.007583	3.904484
C	2.131362	-1.679172	2.478843
C	2.229234	-2.829642	1.464140
C	0.915712	-3.401119	0.909646
C	0.142887	-2.438894	0.007682
H	-0.861075	-2.820823	-0.233799
H	0.684702	-2.259237	-0.938499
H	0.270769	-3.745745	1.732374
H	1.161294	-4.311723	0.329914
H	2.803363	-3.636666	1.950867
H	2.844516	-2.490571	0.613366
H	3.130636	-1.218017	2.549844
H	1.540719	-0.802368	2.095914
H	2.287215	-2.851601	4.257853

H	1.939793	-1.151847	4.548603
H	-0.107335	-3.259200	3.645560
H	0.119319	-2.576295	5.243530
H	-0.383789	-0.241331	4.128393
H	-1.671952	-1.338820	4.567974
H	-1.849120	-2.160909	2.170842
H	-2.229863	-0.441362	2.394398
P	-1.775483	0.266514	-0.627847
C	-2.990262	1.445313	0.064546
C	-4.308173	1.532274	-0.411951
C	-5.182875	2.479524	0.127769
C	-4.750932	3.343074	1.139210
C	-3.438597	3.260505	1.617025
C	-2.562395	2.312630	1.085506
H	-1.540064	2.252068	1.470911
H	-3.099016	3.930755	2.410204
H	-5.439584	4.080109	1.559340
H	-6.207892	2.542521	-0.245407
H	-4.655153	0.860687	-1.200433
C	-2.725306	-1.048526	-1.461519
C	-2.629547	-1.307438	-2.837379
C	-3.343819	-2.370501	-3.400710
C	-4.155271	-3.176465	-2.598817
C	-4.251520	-2.923542	-1.225043
C	-3.535542	-1.870782	-0.655343
H	-3.606078	-1.686950	0.419963
H	-4.883776	-3.552575	-0.593944
H	-4.713231	-4.004270	-3.042968
H	-3.265623	-2.565112	-4.473053
H	-2.004730	-0.689399	-3.484821
C	-0.880444	1.241322	-1.938461
C	0.497795	0.654879	-2.266783
P	1.537186	0.568581	-0.722198
C	1.953245	2.316155	-0.364440
C	1.675791	2.832198	0.912420
C	1.964597	4.166478	1.217300
C	2.533758	4.993678	0.245981
C	2.819985	4.486083	-1.027627
C	2.534016	3.154563	-1.332984
H	2.773609	2.764290	-2.325571
H	3.272167	5.131707	-1.784423
H	2.760388	6.036525	0.480982
H	1.747545	4.557270	2.214288
H	1.242063	2.188599	1.683899
C	3.111520	-0.224420	-1.215846
C	4.297566	0.123998	-0.543595
C	5.486947	-0.557040	-0.812306
C	5.509534	-1.592307	-1.752650
C	4.335602	-1.943291	-2.425197
C	3.141224	-1.268278	-2.157788
H	2.237127	-1.567900	-2.691225
H	4.346068	-2.748409	-3.163978
H	6.441393	-2.122823	-1.962556
H	6.401894	-0.273919	-0.286050
H	4.298720	0.934983	0.188943
H	0.403839	-0.370629	-2.656034
H	1.008709	1.253593	-3.036777
H	-1.514216	1.328492	-2.834387
H	-0.782644	2.258845	-1.527464

H	2.161517	-1.992588	4.063388
H	-0.278556	-3.666879	3.230832
H	0.216571	-3.201496	4.845886
H	0.007931	-0.703956	3.963825
H	-1.374337	-1.609281	4.530336
H	-2.015314	-2.191674	2.118731
H	-2.067910	-0.460008	2.519865
P	-1.815943	0.324674	-0.558083
C	-2.328305	2.000737	-0.026865
C	-3.538768	2.574945	-0.451415
C	-3.866224	3.877345	-0.066745
C	-2.992777	4.616734	0.738455
C	-1.787862	4.050744	1.165870
C	-1.459447	2.746144	0.789774
H	-0.512311	2.316870	1.127393
H	-1.101942	4.622366	1.795573
H	-3.253979	5.635368	1.035362
H	-4.809868	4.317475	-0.398194
H	-4.229522	2.005225	-1.077354
C	-3.342526	-0.602270	-0.918341
C	-3.647286	-1.101279	-2.195332
C	-4.814670	-1.845146	-2.395235
C	-5.682299	-2.094519	-1.328987
C	-5.382626	-1.599168	-0.054673
C	-4.217551	-0.860733	0.153512
H	-3.988958	-0.483100	1.152637
H	-6.057649	-1.792561	0.782350
H	-6.593498	-2.675625	-1.490013
H	-5.045417	-2.228931	-3.391889
H	-2.987143	-0.916907	-3.044397
C	-0.944433	0.588951	-2.180798
C	0.376510	1.349285	-1.990044
P	1.470377	0.589445	-0.677183
C	2.423987	1.995149	0.003647
C	2.345593	2.274048	1.378198
C	3.041112	3.359447	1.921005
C	3.820136	4.171061	1.092300
C	3.909083	3.895323	-0.277888
C	3.217806	2.811589	-0.821767
H	3.302204	2.595301	-1.890037
H	4.523803	4.526737	-0.924005
H	4.364739	5.019260	1.514286
H	2.975964	3.567884	2.991607
H	1.742736	1.640420	2.035641
C	2.697944	-0.443380	-1.559943
C	3.931834	-0.713592	-0.940361
C	4.835000	-1.602541	-1.526334
C	4.516889	-2.236807	-2.732352
C	3.293637	-1.971595	-3.354093
C	2.385971	-1.080763	-2.772448
H	1.435921	-0.889770	-3.276302
H	3.041428	-2.460051	-4.298462
H	5.223696	-2.934348	-3.187880
H	5.792826	-1.799814	-1.038669
H	4.194537	-0.222538	0.000168
H	0.923862	1.424820	-2.942195
H	0.177874	2.377734	-1.650526
H	-0.772927	-0.413297	-2.604978
H	-1.609894	1.136575	-2.866829

H	-2.193434	-1.443627	3.856805
H	-0.828849	0.090366	4.978338
H	0.295880	-1.264541	5.042074
H	1.487151	0.734221	4.270748
H	0.260686	1.093201	3.087654
H	2.465082	0.030233	2.172830
H	1.904218	-1.529875	2.826446
P	-1.624477	0.392135	-0.661302
C	-1.911864	2.192913	-0.435342
C	-2.478250	2.985491	-1.450490
C	-2.651025	4.357323	-1.259381
C	-2.265633	4.954827	-0.052846
C	-1.712310	4.175781	0.965959
C	-1.537472	2.801015	0.774735
H	-1.114636	2.203114	1.586860
H	-1.418427	4.635226	1.912793
H	-2.403121	6.028964	0.093395
H	-3.092050	4.964310	-2.053734
H	-2.795008	2.528863	-2.391769
C	-3.272054	-0.316927	-1.029405
C	-3.402673	-1.449528	-1.852723
C	-4.655172	-2.037090	-2.047800
C	-5.787192	-1.508923	-1.419735
C	-5.663172	-0.386666	-0.594894
C	-4.414311	0.207399	-0.398187
H	-4.334443	1.088981	0.242433
H	-6.544033	0.033141	-0.102932
H	-6.765311	-1.970924	-1.573772
H	-4.745139	-2.912939	-2.694925
H	-2.532153	-1.886467	-2.346414
C	-0.688002	0.308312	-2.273227
C	0.703234	0.932517	-2.113826
P	1.673451	0.158791	-0.727423
C	2.902567	1.430571	-0.266782
C	4.263660	1.333212	-0.591816
C	5.147200	2.342441	-0.195624
C	4.680916	3.447890	0.521291
C	3.323024	3.548972	0.846120
C	2.437652	2.542669	0.459108
H	1.378496	2.626086	0.720580
H	2.954687	4.410879	1.407660
H	5.376243	4.232050	0.830244
H	6.206611	2.262215	-0.451067
H	4.638636	0.473311	-1.150382
C	2.581231	-1.273448	-1.403622
C	3.361422	-2.029610	-0.508377
C	4.042477	-3.162053	-0.955582
C	3.938567	-3.562482	-2.292909
C	3.155556	-2.822861	-3.182340
C	2.479244	-1.679902	-2.742979
H	1.874589	-1.118432	-3.457548
H	3.069786	-3.132476	-4.226699
H	4.466888	-4.453808	-2.639821
H	4.651610	-3.739112	-0.255800
H	3.434418	-1.732272	0.540668
H	1.281460	0.892320	-3.049553
H	0.621569	1.998682	-1.848552
H	-0.612065	-0.752816	-2.556936
H	-1.258138	0.818288	-3.065083

^{4}10A-20
Geometry with 77 atoms:
Total energy: -3045.619444410

Cr	-0.153844	-0.793924	0.856926
C	-1.387890	-1.326189	2.393769
C	-0.631921	-1.575334	3.710379
C	0.216557	-2.861599	3.797058
C	1.694673	-2.735165	3.391541
C	2.058787	-2.353792	1.950851
C	1.852919	-3.399851	0.845600
C	0.412045	-3.655617	0.384017
C	-0.236526	-2.461752	-0.318636
H	-1.294251	-2.666441	-0.553376
H	0.296444	-2.223725	-1.257663
H	-0.212589	-3.980648	1.230342
H	0.427006	-4.514591	-0.314381
H	2.301323	-4.343569	1.201089
H	2.446095	-3.091595	-0.032424
H	3.122526	-2.063506	1.942807
H	1.583615	-1.368175	1.688967
H	2.202974	-3.691026	3.608922

^{4}10A-21
Geometry with 77 atoms:
Total energy: -3045.616933500

Cr	0.121821	-0.564732	1.035646
C	1.573193	-0.536717	2.484604
C	0.798242	0.237101	3.562881
C	-0.233165	-0.589555	4.348354
C	-1.164489	-1.439437	3.459629
C	-0.701685	-2.890104	3.263658
C	-1.436430	-3.688840	2.181362
C	-1.444163	-3.053641	0.779783
C	-0.110311	-2.467873	0.301135
H	-0.076420	-2.394748	-0.799381
H	0.764136	-3.062271	0.617011
H	-2.232714	-2.279665	0.731119
H	-1.787999	-3.821078	0.061128
H	-2.480649	-3.869292	2.491548
H	-0.960070	-4.682569	2.122349
H	-0.815224	-3.404589	4.232972
H	0.377618	-2.905372	3.051856
H	-1.331055	-0.914539	2.477845

^{4}10A-22
Geometry with 77 atoms:
Total energy: -3045.616859520

Cr	0.095526	-0.594796	0.987880
C	-0.105389	-2.460748	0.204179
C	-0.962183	-3.351143	1.107375
C	-2.262585	-2.696265	1.594738
C	-2.065030	-1.579439	2.627837
C	-1.508871	-2.030387	3.995660
C	-0.263241	-1.295046	4.515271
C	1.063655	-1.593725	3.787355
C	1.392955	-0.749945	2.550831
H	2.408129	-0.991139	2.189637
H	1.419874	0.332765	2.824190
H	1.096638	-2.667665	3.527121
H	1.879455	-1.454840	4.522187
H	-0.141599	-1.575995	5.574259
H	-0.446558	-0.203046	4.520923
H	-1.280436	-3.108760	3.958828
H	-2.311761	-1.925113	4.743127
H	-3.017845	-1.042689	2.763088

H	-1.425518	-0.745267	2.231713
H	-2.910346	-3.458631	2.060578
H	-2.823540	-2.304681	0.730173
H	-1.218157	-4.279010	0.561621
H	-0.365953	-3.680723	1.975612
H	0.905303	-2.875173	0.064010
H	-0.568170	-2.339683	-0.792957
P	-1.550190	0.507122	-0.731947
C	-1.928114	2.275570	-0.430521
C	-2.582629	3.066118	-1.392476
C	-2.817542	4.419964	-1.147454
C	-2.404042	4.999628	0.058549
C	-1.758994	4.221747	1.023097
C	-1.523302	2.864354	0.779512
H	-1.026859	2.265170	1.548584
H	-1.441348	4.668728	1.968187
H	-2.590241	6.059841	0.246620
H	-3.327442	5.027061	-1.899414
H	-2.918703	2.621730	-2.332877
C	-3.138092	-0.278423	-1.181965
C	-3.182311	-1.363278	-2.075702
C	-4.385146	-2.036328	-2.307054
C	-5.551920	-1.642125	-1.645641
C	-5.513709	-0.566748	-0.752062
C	-4.315632	0.111817	-0.518520
H	-4.302413	0.952665	0.179440
H	-6.422785	-0.251227	-0.234144
H	-6.490617	-2.170868	-1.827635
H	-4.408322	-2.873799	-3.008591
H	-2.282785	-1.694982	-2.598208
C	-0.534338	0.544685	-2.294517
C	0.841357	1.152978	-2.001206
P	1.756142	0.222484	-0.673662
C	2.993236	1.416594	-0.048230
C	4.370423	1.286992	-0.282832
C	5.258396	2.234238	0.237053
C	4.781597	3.312360	0.987457
C	3.408231	3.448005	1.220680
C	2.517620	2.502899	0.710534
H	1.446180	2.620274	0.898275
H	3.030626	4.290021	1.805727
H	5.480130	4.048626	1.392261
H	6.329723	2.127472	0.050257
H	4.755367	0.450534	-0.869191
C	2.659125	-1.140371	-1.488416
C	3.426872	-1.997238	-0.676624
C	4.105056	-3.079255	-1.238168
C	4.010876	-3.330508	-2.611864
C	3.240825	-2.491925	-3.420939
C	2.567468	-1.398846	-2.865388
H	1.975633	-0.758494	-3.521493
H	3.162803	-2.684562	-4.493640
H	4.536850	-4.182106	-3.050034
H	4.704108	-3.732849	-0.599748
H	3.495375	-1.817828	0.398655
H	1.464563	1.221088	-2.905732
H	0.739025	2.181485	-1.621457
H	-0.436157	-0.491203	-2.654603
H	-1.061841	1.116651	-3.073647

[4]10A-23
Geometry with 77 atoms:
Total energy: -3045.616507950

Cr	-0.151406	-0.713458	0.916652
C	-1.262738	-0.702695	2.618261
C	-1.034845	-1.669096	3.785452
C	0.389056	-1.768807	4.369626
C	1.356949	-2.713184	3.639258
C	1.920967	-2.209959	2.296759
C	1.907289	-3.230518	1.153418
C	0.501695	-3.607282	0.668472
C	-0.211379	-2.486915	-0.091533
H	-1.259859	-2.752715	-0.299779
H	0.293813	-2.288804	-1.055001
H	-0.116238	-3.929599	1.524981
H	0.578782	-4.496095	0.014025
H	2.436186	-4.131405	1.509595
H	2.494573	-2.843769	0.303593
H	2.941750	-1.817967	2.434547
H	1.382449	-1.267528	2.009594
H	0.844321	-3.677178	3.485775
H	2.207949	-2.934206	4.303730
H	0.301493	-2.128430	5.407842
H	0.832685	-0.757131	4.444369
H	-1.705750	-1.366766	4.612036
H	-1.375176	-2.681282	3.497736
H	-2.341723	-0.614323	2.406227
H	-0.930039	0.327701	2.905007
P	-1.809032	0.296474	-0.598332
C	-2.389047	1.954549	-0.071036
C	-1.447696	2.850788	0.471166
C	-1.840634	4.124884	0.884428
C	-3.180337	4.513016	0.777249
C	-4.123273	3.622382	0.256202
C	-3.734013	2.347928	-0.167000
H	-4.482553	1.662195	-0.568627
H	-5.172254	3.918367	0.178447
H	-3.489988	5.507961	1.106169
H	-1.098283	4.812305	1.297200
H	-0.398637	2.563109	0.575240
C	-3.289296	-0.684643	-1.028016
C	-3.944861	-0.530704	-2.262946
C	-5.080101	-1.291336	-2.553718
C	-5.571996	-2.206883	-1.617756
C	-4.925395	-2.363590	-0.388228
C	-3.787253	-1.609301	-0.093545
H	-3.279113	-1.747331	0.861993
H	-5.303913	-3.080316	0.344400
H	-6.459794	-2.800594	-1.848917
H	-5.583066	-1.166371	-3.515620
H	-3.580324	0.184331	-3.003061
C	-0.918593	0.563642	-2.217514
C	0.442284	1.256143	-2.060373
P	1.534862	0.501353	-0.738503
C	2.508160	1.920405	-0.114299
C	2.381585	2.294672	1.233860
C	3.070995	3.407251	1.727487
C	3.893529	4.150025	0.876635
C	4.030738	3.779089	-0.466884
C	3.343929	2.669654	-0.962181
H	3.463771	2.380826	-2.009430
H	4.678164	4.357240	-1.130718
H	4.433600	5.019130	1.260150
H	2.966831	3.690156	2.777683
H	1.742526	1.717056	1.908246
C	2.728230	-0.574338	-1.613890
C	2.339686	-1.311505	-2.746009
C	3.222552	-2.224804	-3.329507
C	4.497292	-2.415371	-2.788767
C	4.889085	-1.687109	-1.660424
C	4.010834	-0.774468	-1.071881
H	4.330886	-0.210882	-0.191801
H	5.886062	-1.828003	-1.235782
H	5.185959	-3.129324	-3.246666
H	2.910924	-2.789015	-4.211884
H	1.346355	-1.184107	-3.181959
H	0.979879	1.267209	-3.021259
H	0.299762	2.306235	-1.762781
H	-0.815977	-0.440847	-2.659238
H	-1.560130	1.154232	-2.889803

[4]10A-24
Geometry with 77 atoms:
Total energy: -3045.616555230

Cr	0.196041	-0.677934	1.022287
C	1.477714	-0.760979	2.609779
C	1.087498	-1.770735	3.695334
C	-0.372137	-1.650479	4.151685
C	-1.406633	-1.907174	3.052718
C	-1.513558	-3.344547	2.522458
C	-2.086674	-3.409800	1.096874
C	-1.036869	-3.347966	-0.038627
C	0.248612	-2.550015	0.198657
H	0.833713	-2.497465	-0.736388
H	0.903423	-3.036163	0.944687
H	-1.536476	-2.985024	-0.950453
H	-0.727464	-4.386504	-0.268222
H	-2.819455	-2.592617	0.973690
H	-2.669045	-4.335746	0.968938
H	-2.158264	-3.903697	3.219856
H	-0.533412	-3.845186	2.557558
H	-1.265738	-1.195581	2.189708
H	-2.404769	-1.579162	3.389559
H	-0.534042	-0.640201	4.568774
H	-0.570065	-2.356636	4.976597
H	1.282589	-2.795419	3.332747
H	1.739434	-1.649765	4.581249
H	1.372903	0.283136	2.988717
H	2.530375	-0.891883	2.310780
P	-1.509300	0.495320	-0.630198
C	-2.406660	1.947862	0.035026
C	-3.245973	2.728253	-0.780052
C	-3.877983	3.857574	-0.257112
C	-3.682856	4.217121	1.082223
C	-2.857261	3.442932	1.901638
C	-2.222282	2.310998	1.379972
H	-1.586801	1.706583	2.034499
H	-2.709787	3.715491	2.949428
H	-4.181480	5.100797	1.487899
H	-4.528708	4.459809	-0.895828
H	-3.412619	2.447958	-1.823412
C	-2.779801	-0.500306	-1.497590
C	-2.523229	-1.107453	-2.738663
C	-3.475363	-1.949001	-3.321696
C	-4.688855	-2.195497	-2.673418
C	-4.951238	-1.592869	-1.438565
C	-4.002974	-0.753177	-0.850948
H	-4.222972	-0.285808	0.112378
H	-5.900060	-1.776905	-0.928723
H	-5.430800	-2.854417	-3.130620
H	-3.265452	-2.414372	-4.287844
H	-1.579182	-0.937822	-3.261016
C	-0.425067	1.206595	-1.980033
C	0.861512	0.395307	-2.186688
P	1.809136	0.247765	-0.591065
C	2.383721	1.953681	-0.260345
C	3.579792	2.457573	-0.799419
C	3.942983	3.787184	-0.571783
C	3.117499	4.624835	0.186404
C	1.923846	4.131202	0.721335
C	1.560770	2.800042	0.503303
H	0.622116	2.429864	0.923236
H	1.273703	4.780131	1.312906
H	3.406465	5.664016	0.361340
H	4.876250	4.171278	-0.990667
H	4.231718	1.812452	-1.392695
C	3.288531	-0.760269	-0.933370
C	4.326183	-0.769888	0.017966
C	5.444331	-1.583122	-0.169855
C	5.536484	-2.401077	-1.301614
C	4.508060	-2.398972	-2.247179
C	3.386098	-1.583846	-2.066981
H	2.597646	-1.599228	-2.820797
H	4.575968	-3.033759	-3.133850
H	6.411557	-3.039127	-1.446145
H	6.246643	-1.579213	0.571857
H	4.267151	-0.131478	0.902785
H	0.630463	-0.628484	-2.520444
H	1.504834	0.862332	-2.949237
H	-0.995450	1.282621	-2.918322
H	-0.186778	2.235421	-1.669054

[4]10A-25(10')
Geometry with 77 atoms:
Total energy: -3045.615287740

Cr	-0.055939	-0.585815	0.956540
C	-1.157236	-2.338316	0.798537
C	-0.499485	-2.665878	2.103452
C	-1.366496	-2.655053	3.375329
C	-2.372886	-1.498712	3.511275
C	-1.895561	-0.057632	3.268691
C	-0.795611	0.533517	4.162851
C	0.642766	0.058066	3.910450
C	1.137868	0.250984	2.470558
H	2.193345	-0.059096	2.383609
H	1.114738	1.324355	2.188470
H	0.749524	-0.999415	4.205771
H	1.302985	0.612391	4.605076
H	-1.067748	0.354359	5.217967
H	-0.815652	1.630162	4.029841
H	-2.785952	0.588706	3.345318
H	-1.616336	0.074735	2.193586
H	-2.805713	-1.547016	4.525013

H -3.215942 -1.680338 2.823281
H -0.699042 -2.679617 4.251560
H -1.936569 -3.598734 3.404779
H 0.097614 -3.592420 2.059984
H 0.343835 -1.905053 2.296566
H -0.821568 -2.934813 -0.062632
H -2.249935 -2.252104 0.811269
P 1.767187 -0.017757 -0.659551
C 2.677897 -1.517440 -1.184799
C 3.567208 -1.485703 -2.274636
C 4.248937 -2.641835 -2.657259
C 4.051695 -3.838696 -1.957717
C 3.174283 -3.877182 -0.871080
C 2.490307 -2.720476 -0.485057
H 1.808475 -2.755933 0.367982
H 3.020371 -4.808608 -0.321165
H 4.587146 -4.741889 -2.260533
H 4.940060 -2.609094 -3.503031
H 3.741584 -0.553890 -2.818739
C 3.023543 1.229413 -0.198882
C 2.623590 2.570006 -0.046113
C 3.534759 3.530946 0.395087
C 4.849763 3.164253 0.701138
C 5.249037 1.832201 0.563734
C 4.342275 0.865408 0.118511
H 4.668967 -0.171450 0.017090
H 6.274171 1.539518 0.803499
H 5.561342 3.916628 1.049658
H 3.214436 4.570033 0.503831
H 1.596660 2.872700 -0.265154
C 0.976453 0.630295 -2.221822
C -0.393789 -0.020101 -2.445544
P -1.447255 0.212451 -0.930721
C -3.067324 -0.550775 -1.286500
C -3.236974 -1.528688 -2.279077
C -4.480353 -2.146936 -2.449274
C -5.558389 -1.798990 -1.631819
C -5.394004 -0.825943 -0.638981
C -4.156115 -0.205998 -0.464221
H -4.039165 0.556541 0.310999
H -6.234842 -0.547228 0.000825
H -6.527989 -2.283921 -1.768129
H -4.603889 -2.903609 -3.227955
H -2.409000 -1.818842 -2.928469
C -1.769291 2.019841 -0.897190
C -2.539251 2.635595 -1.900372
C -2.740836 4.016672 -1.879867
C -2.180399 4.795269 -0.859568
C -1.419335 4.190083 0.143852
C -1.215079 2.806253 0.126310
H -0.620158 2.342676 0.916824
H -0.985689 4.792269 0.945848
H -2.344072 5.875574 -0.845479
H -3.341531 4.488660 -2.661158
H -2.992451 2.034079 -2.692697
H -0.900438 0.409683 -3.323844
H -0.287300 -1.103919 -2.614323
H 0.873527 1.720710 -2.109393
H 1.643953 0.455680 -3.078804

^{4}10B-01
Geometry with 85 atoms:
Total energy: -3274.529005580
Cr -0.425211 -0.839517 0.850253
C 0.701078 -1.616462 2.394963
C -0.158042 -2.487279 3.324570
C -1.389575 -1.767920 3.892953
C -2.442004 -1.269781 2.887789
C -3.448658 -2.285652 2.332777
H -3.963716 -2.726188 3.204709
H -4.224721 -1.725345 1.780920
C -2.960924 -3.429868 1.430937
C -2.414171 -3.036619 0.046126
C -0.939371 -2.619384 -0.030716
H -0.307645 -3.393841 0.438463
H -0.622637 -2.544150 -1.087405
H -2.544931 -3.915305 -0.614577
H -3.067698 -2.259865 -0.389980
H -3.832860 -4.086217 1.271480
H -2.220355 -4.051622 1.960245
H -1.983347 -0.692201 2.042490
H -3.024414 -0.466578 3.370217
H -1.036835 -0.901143 4.479490
H -1.906779 -2.423165 4.615442
H 0.447844 -2.840845 4.181509
H -0.469391 -3.402831 2.797445
H 1.541043 -2.211065 1.997017
H 1.157289 -0.777879 2.955081
P -1.594326 0.428616 -1.009512
C -3.281703 0.171809 -1.653941
C -3.524312 -0.544827 -2.837458
C -4.836650 -0.829256 -3.228573
C -5.913515 -0.405281 -2.445837
C -5.677440 0.309706 -1.265878
C -4.370435 0.594135 -0.868527
H -4.196434 1.150191 0.056825
H -6.516049 0.646383 -0.651413
H -6.937307 -0.630366 -2.754076
H -5.015655 -1.386000 -4.151675
H -2.698108 -0.893194 -3.460456
C -1.509128 2.188123 -0.513672
C -1.923268 3.218807 -1.372352
C -1.810301 4.557471 -0.999198
C -1.275623 4.870994 0.253409
C -0.862298 3.865130 1.130166
C -0.978838 2.519396 0.752061
O -0.579756 1.486251 1.576072
C -0.164356 1.813124 2.911077
H -0.957002 2.370356 3.434019
H 0.010325 0.864867 3.426289
H 0.770387 2.393139 2.896460
H -0.442623 4.142539 2.095268
H -1.177326 5.914709 0.561601
H -2.137761 5.348521 -1.676827
H -2.349322 2.959995 -2.345385
C -0.438261 0.323524 -2.460041
C 0.984569 0.713605 -2.038651
P 1.549210 -0.178704 -0.490331
C 2.530932 1.011240 0.507749
C 3.415025 0.483010 1.465441
C 4.121064 1.332741 2.319361
C 3.950453 2.718853 2.233168
C 3.069690 3.248781 1.285927
C 2.361302 2.401239 0.428545
H 1.673684 2.844485 -0.291812
H 2.929387 4.329924 1.208490
H 4.504578 3.383289 2.900682
H 4.808807 0.908773 3.055132
H 3.556800 -0.597144 1.543830
C 2.749891 -1.436647 -1.040678
C 2.566538 -2.793835 -0.743504
C 3.507862 -3.748156 -1.138684
C 4.647197 -3.338949 -1.833711
C 4.855922 -1.990851 -2.142268
C 3.909390 -1.033085 -1.752809
O 4.015870 0.288526 -2.013192
C 5.194697 0.809042 -2.608166
H 6.086385 0.584437 -1.998477
H 5.057713 1.897544 -2.655543
H 5.340366 0.419410 -3.630362
H 5.752111 -1.694206 -2.687062
H 5.392104 -4.075451 -2.145406
H 3.351368 -4.801925 -0.899850
H 1.680121 -3.105862 -0.193335
H 1.706399 0.501163 -2.837982
H 1.036263 1.794508 -1.847312
H -0.468317 -0.718642 -2.817495
H -0.789268 0.967061 -3.282264

^{4}10B-02
Geometry with 85 atoms:
Total energy: -3274.530201490
Cr 0.250468 -0.276939 1.108493
C 0.278589 1.589778 1.940827
C -0.988935 1.869657 2.753700
C -1.216484 0.819884 3.847927
C -1.678751 -0.539685 3.310767
C -1.389023 -1.746223 4.202896
H -1.884061 -1.573680 5.174920
H -1.878655 -2.636450 3.768120
C 0.093160 -2.068499 4.450498
C 0.933781 -2.444914 3.215035
C 1.525628 -1.287756 2.388307
H 2.019483 -0.564802 3.061512
H 2.311548 -1.691881 1.722943
H 1.773870 -3.068562 3.575731
H 0.341822 -3.128080 2.577028
H 0.120243 -2.914429 5.157605
H 0.582266 -1.230871 4.977560
H -1.257303 -0.768235 2.295716
H -2.757305 -0.490147 3.084294
H -1.972786 1.167638 4.571641
H -0.279857 0.701781 4.416624
H -1.872590 1.914411 2.089014
H -0.922338 2.870123 3.222815
H 1.175716 1.641866 2.581802
H 0.397567 2.318694 1.127297
P -1.501425 0.289685 -0.840038
C -2.602840 -1.148541 -1.158795
C -2.743090 -1.770520 -2.409690
C -3.568639 -2.891190 -2.553569
C -4.273803 -3.395455 -1.456886
C -4.155697 -2.771653 -0.210168
C -3.322900 -1.660849 -0.062976
H -3.231316 -1.186229 0.916999
H -4.709283 -3.153635 0.651150
H -4.918654 -4.269694 -1.574285
H -3.666438 -3.366901 -3.532561
H -2.217556 -1.388449 -3.286761
C -2.661711 1.721892 -0.920284
C -4.050226 1.547697 -1.027086
C -4.925075 2.637185 -0.984891
C -4.412752 3.925126 -0.832515
C -3.033621 4.131235 -0.734087
C -2.158021 3.038585 -0.783807
O -0.807483 3.161269 -0.721519
C -0.218844 4.429662 -0.472639
H -0.561104 4.850928 0.487599
H 0.865779 4.264624 -0.421487
H -0.434672 5.142278 -1.287033
H -2.647738 5.143937 -0.623001
H -5.085701 4.785252 -0.793219
H -6.001348 2.473401 -1.070105
H -4.462904 0.544795 -1.141837
C -0.404196 0.379200 -2.355884
C 0.954878 1.040980 -2.095848
P 1.833803 0.280009 -0.648000
C 3.307031 1.304914 -0.339838
C 4.009794 1.102490 0.861775
C 5.145629 1.862153 1.145657
C 5.585128 2.834454 0.240548
C 4.886812 3.044632 -0.951827
C 3.751376 2.283257 -1.246042
H 3.223821 2.460249 -2.185111
H 5.228084 3.802457 -1.661240
H 6.472503 3.430745 0.466562
H 5.686456 1.697792 2.080640
H 3.666267 0.352062 1.576216
C 2.422509 -1.328910 -1.289660
C 3.615817 -1.467229 -2.011340
C 4.010037 -2.712027 -2.506395
C 3.200822 -3.826506 -2.277911
C 2.008321 -3.714172 -1.555322
C 1.620089 -2.465888 -1.054538
O 0.466232 -2.274624 -0.324427
C -0.365961 -3.411326 -0.061714
H -1.182532 -3.062692 0.577117
H 0.197178 -4.197114 0.463235
H -0.791232 -3.805248 -0.997363
H 1.401564 -4.602773 -1.389333
H 3.496640 -4.806127 -2.660911
H 4.943595 -2.810327 -3.064022
H 4.246402 -0.590174 -2.178212
H 1.596547 0.945308 -2.985826
H 0.827837 2.106383 -1.868805
H -0.248377 -0.664321 -2.671814
H -0.931319 0.895422 -3.172259

^{4}10B-03
Geometry with 85 atoms:
Total energy: -3274.530670580
Cr 0.147157 -0.567532 0.997033
C -0.092575 0.870946 2.432612

C	-1.383218	0.624991	3.224790
C	-1.455623	-0.794666	3.803336
C	-1.734088	-1.871790	2.747739
C	-1.303073	-3.298074	3.090972
H	-1.885010	-3.616226	3.974129
H	-1.616767	-3.966969	2.269263
C	0.187639	-3.527596	3.380647
C	1.180370	-3.236855	2.242359
C	1.538875	-1.763268	1.983722
H	1.792788	-1.269383	2.938626
H	2.456889	-1.733530	1.370088
H	2.113497	-3.777104	2.491727
H	0.824776	-3.722119	1.314191
H	0.294357	-4.587754	3.666985
H	0.491202	-2.953670	4.273353
H	-1.301773	-1.614354	1.743782
H	-2.808128	-1.868401	2.499873
H	-2.245916	-0.865293	4.569620
H	-0.506593	-1.006172	4.321239
H	-2.268366	0.810144	2.585637
H	-1.464245	1.355589	4.051894
H	0.783513	0.831069	3.102963
H	-0.104159	1.854380	1.944244
P	-1.485470	0.619675	-0.755432
C	-2.925687	-0.417527	-1.227429
C	-3.193550	-0.846682	-2.537333
C	-4.271806	-1.700865	-2.794652
C	-5.100208	-2.126997	-1.753074
C	-4.852584	-1.690383	-0.446603
C	-3.771426	-0.846622	-0.186499
H	-3.588196	-0.508694	0.836117
H	-5.501296	-2.010155	0.372627
H	-5.941430	-2.793269	-1.958884
H	-4.467246	-2.028591	-3.818703
H	-2.571303	-0.520873	-3.372234
C	-2.212626	2.297756	-0.520572
C	-3.585992	2.542759	-0.676358
C	-4.134177	3.800190	-0.408451
C	-3.304061	4.834184	0.023957
C	-1.930809	4.623318	0.178182
C	-1.381372	3.364851	-0.098861
O	-0.053861	3.092282	0.002076
C	0.837569	4.063493	0.533295
H	0.545069	4.362596	1.553738
H	1.825754	3.587353	0.570167
H	0.890146	4.957151	-0.111738
H	-1.294584	5.442848	0.510687
H	-3.720704	5.820468	0.242600
H	-5.206016	3.965123	-0.536711
H	-4.244842	1.738466	-1.006971
C	-0.448330	0.704338	-2.309152
C	0.983507	1.192110	-2.056837
P	1.764765	0.298704	-0.621830
C	3.245951	1.251814	-0.166748
C	3.681785	1.206437	1.169128
C	4.801185	1.942326	1.565264
C	5.487088	2.731751	0.636686
C	5.054049	2.785182	-0.692585
C	3.937683	2.048958	-1.097051
H	3.610223	2.104130	-2.137595
H	5.587023	3.403518	-1.418943
H	6.360165	3.309758	0.949451
H	5.134638	1.902754	2.604881
H	3.142223	0.601308	1.900178
C	2.321180	-1.276479	-1.389657
C	3.578374	-1.444106	-1.983244
C	3.934255	-2.660170	-2.573298
C	3.024951	-3.718535	-2.569655
C	1.766636	-3.579297	-1.973293
C	1.420692	-2.363223	-1.378918
O	0.205600	-2.156226	-0.748533
C	-0.826635	-3.142148	-0.889001
H	-1.066288	-3.298004	-1.951871
H	-1.709689	-2.743739	-0.378635
H	-0.532414	-4.094980	-0.424151
H	1.077909	-4.422974	-1.970430
H	3.292050	-4.673461	-3.028322
H	4.918706	-2.778214	-3.030703
H	4.290955	-0.615975	-1.977656
H	1.601346	1.025989	-2.952491
H	0.997934	2.261305	-1.816337
H	-0.422533	-0.324374	-2.701699
H	-0.942454	1.336261	-3.062699

^{4}10B-04

Geometry with 85 atoms:

Total energy: -3274.530512670

Cr	-0.391893	-0.432918	0.918598
C	-0.190960	-2.406812	0.361682
C	0.868766	-3.142352	1.192919
C	0.723355	-2.883366	2.696030
C	1.162589	-1.477226	3.118970
C	0.642193	-0.997978	4.474584
H	1.067285	-1.661727	5.248229
H	1.056252	0.005583	4.681836
C	-0.883422	-0.956859	4.651375
C	-1.670807	-0.035576	3.703919
C	-1.951658	-0.557298	2.283147
H	-2.331499	-1.593546	2.318148
H	-2.762324	0.052570	1.843747
H	-2.642729	0.167449	4.193268
H	-1.172197	0.952551	3.671163
H	-1.074806	-0.631017	5.687781
H	-1.298232	-1.977162	4.584431
H	0.916305	-0.694500	2.350715
H	2.263529	-1.422351	3.100381
H	1.324492	-3.605283	3.275335
H	-0.325393	-3.056824	2.983947
H	1.879880	-2.845012	0.871856
H	0.801920	-4.230657	1.005805
H	-1.185949	-2.859284	0.517669
H	0.045802	-2.487283	-0.714545
P	-1.904959	-0.004672	-0.893738
C	-3.380372	-1.042576	-1.125489
C	-3.298740	-2.216341	-1.896210
C	-4.401017	-3.068759	-1.993492
C	-5.586925	-2.765647	-1.317792
C	-5.668483	-1.606646	-0.539567
C	-4.571494	-0.748598	-0.437714
H	-4.648041	0.152599	0.173528
H	-6.591748	-1.366874	-0.006618
H	-6.447351	-3.434568	-1.395683
H	-4.330506	-3.975294	-2.599239
H	-2.377545	-2.478536	-2.420551
C	-2.457480	1.720937	-0.658974
C	-3.491037	2.290279	-1.418271
C	-3.852012	3.627444	-1.248398
C	-3.167815	4.405609	-0.311652
C	-2.131467	3.864111	0.454203
C	-1.774565	2.520561	0.283615
O	-0.756366	1.926566	0.996307
C	-0.004026	2.723886	1.917533
H	0.520396	3.536017	1.391957
H	-0.652356	3.132056	2.707768
H	0.736884	2.057570	2.371366
H	-1.616091	4.497276	1.174616
H	-3.438849	5.454312	-0.167970
H	-4.660443	4.058508	-1.842197
H	-4.023323	1.670954	-2.144791
C	-0.975721	0.037930	-2.498756
C	0.290337	0.892060	-2.342741
P	1.375104	0.324204	-0.932575
C	2.512821	1.748972	-0.666788
C	3.052804	1.952589	0.614377
C	3.914333	3.023448	0.862210
C	4.245666	3.908201	-0.169123
C	3.716698	3.712589	-1.448398
C	2.858573	2.637504	-1.698631
H	2.469096	2.496406	-2.708737
H	3.977357	4.396731	-2.259693
H	4.918636	4.747388	0.023452
H	4.329562	3.166957	1.863046
H	2.809452	1.258121	1.420258
C	2.420704	-0.993366	-1.671665
C	2.243878	-1.509113	-2.962270
C	3.034705	-2.562502	-3.433271
C	4.017229	-3.108413	-2.606899
C	4.216631	-2.612656	-1.314559
C	3.420463	-1.560363	-0.846380
O	3.527007	-1.020209	0.394229
C	4.559658	-1.444506	1.267202
H	4.495566	-0.807777	2.159599
H	5.554740	-1.312026	0.809475
H	4.431069	-2.498809	1.567244
H	4.986205	-3.052398	-0.680426
H	4.640338	-3.931636	-2.964695
H	2.882172	-2.949964	-4.442746
H	1.483502	-1.091764	-3.624310
H	0.852564	0.922999	-3.288083
H	0.019439	1.933548	-2.106739
H	-0.726114	-1.001302	-2.763283
H	-1.629236	0.437191	-3.290611

^{4}10B-05

Geometry with 85 atoms:

Total energy: -3274.530461160

Cr	-0.312663	-0.824034	0.592950
C	-0.112995	-2.492106	-0.617975
C	1.055547	-3.402543	-0.216389
C	1.067144	-3.710465	1.283834
C	1.486458	-2.505961	2.130440
C	1.091302	-2.538141	3.605582
H	1.610305	-3.393782	4.072990
H	1.495056	-1.635659	4.100217
C	-0.409194	-2.647534	3.916377
C	-1.309092	-1.504862	3.414499
C	-1.725729	-1.537889	1.932767
H	-2.044098	-2.553814	1.640855
H	-2.608687	-0.886420	1.798621
H	-2.226596	-1.525795	4.033234
H	-0.831576	-0.538605	3.668494
H	-0.503438	-2.704576	5.014088
H	-0.804475	-3.606293	3.538915
H	1.136910	-1.536222	1.686608
H	2.574822	-2.366293	2.038604
H	1.763857	-4.536798	1.506551
H	0.067294	-4.063246	1.583568
H	2.018705	-2.943163	-0.499587
H	1.001225	-4.352826	-0.780584
H	-1.070576	-3.029471	-0.500957
H	-0.035080	-2.222879	-1.686263
P	-1.924140	0.209710	-0.865402
C	-3.333253	-0.778037	-1.457365
C	-3.243754	-1.460984	-2.683009
C	-4.271134	-2.317620	-3.085602
C	-5.389592	-2.506136	-2.268338
C	-5.477134	-1.839053	-1.042123
C	-4.453605	-0.982383	-0.631704
H	-4.531661	-0.470853	0.329697
H	-6.347385	-1.986591	-0.398164
H	-6.192557	-3.175667	-2.585837
H	-4.194587	-2.841250	-4.041474
H	-2.371608	-1.337048	-3.329249
C	-2.585516	1.585828	0.142397
C	-3.751872	2.289687	-0.191773
C	-4.201819	3.347037	0.601093
C	-3.478140	3.706641	1.740354
C	-2.310193	3.024091	2.094237
C	-1.863976	1.964014	1.297999
O	-0.709141	1.265467	1.574869
C	0.204993	1.774662	2.553744
H	0.480782	2.813947	2.321409
H	-0.221814	1.708030	3.565907
H	1.103127	1.147466	2.491428
H	-1.763136	3.323258	2.987477
H	-3.822346	4.530161	2.370482
H	-5.112463	3.885621	0.331304
H	-4.317521	1.997851	-1.079853
C	-1.102986	1.003769	-2.355276
C	0.325480	0.489316	-2.599948
P	1.322854	0.457522	-1.021145
C	1.867974	2.208340	-0.815975
C	3.204700	2.603655	-0.992496
C	3.579301	3.937777	-0.809342
C	2.627895	4.898414	-0.453439
C	1.293934	4.517030	-0.281784
C	0.918983	3.182168	-0.455040
H	-0.123749	2.908323	-0.301332
H	0.538875	5.257644	-0.006306
H	2.924932	5.940515	-0.312435
H	4.623589	4.227779	-0.950609
H	3.961860	1.872279	-1.280372
C	2.846352	-0.469480	-1.406123

C 3.137352 -1.043870 -2.649599
C 4.288523 -1.817862 -2.829154
C 5.161813 -2.013484 -1.758563
C 4.899750 -1.443281 -0.507617
C 3.741682 -0.678140 -0.328325
O 3.387874 -0.089910 0.845350
C 4.293807 -0.085225 1.936712
H 3.810349 0.488100 2.738916
H 5.244085 0.406414 1.666988
H 4.502813 -1.104456 2.304690
H 5.595773 -1.603650 0.315432
H 6.064684 -2.614482 -1.891119
H 4.501286 -2.260718 -3.804274
H 2.466448 -0.890960 -3.496425
H 0.295648 -0.547679 -2.966600
H 0.827835 1.103619 -3.362846
H -1.732786 0.851794 -3.244389
H -1.098801 2.086037 -2.160587

^{4}10B-06
Geometry with 85 atoms:
Total energy: -3274.530443650
Cr -0.316820 -0.810451 0.572247
C -0.110623 -2.466855 -0.654057
C 1.034446 -3.397896 -0.231294
C 0.986012 -3.752943 1.258003
C 1.390865 -2.587753 2.162978
C 0.950312 -2.679119 3.621758
H 1.418937 -3.576547 4.063410
H 1.369594 -1.817745 4.173280
C -0.564621 -2.737997 3.870395
C -1.394512 -1.542810 3.368066
C -1.772273 -1.523854 1.874584
H -2.111306 -2.522181 1.547338
H -2.635066 -0.846265 1.741152
H -2.329092 -1.532143 3.960578
H -0.879081 -0.605642 3.656535
H -0.706641 -2.824737 4.960922
H -0.982798 -3.667011 3.445924
H 1.034280 -1.604010 1.762189
H 2.481166 -2.445923 2.103952
H 1.660719 -4.598145 1.477790
H -0.030061 -4.097468 1.508802
H 2.011705 -2.939425 -0.464028
H 0.995104 -4.330503 -0.825621
H -1.077833 -2.993388 -0.573113
H 0.004008 -2.183451 -1.715252
P -1.905516 0.247869 -0.890139
C -3.315488 -0.729220 -1.497518
C -3.221964 -1.403098 -2.727867
C -4.247903 -2.256913 -3.140136
C -5.368963 -2.451826 -2.327980
C -5.460916 -1.793365 -1.097447
C -4.439052 -0.939445 -0.677508
H -4.520082 -0.435715 0.287690
H -6.333074 -1.946005 -0.457258
H -6.170399 -3.119751 -2.652648
H -4.167937 -2.773735 -4.099408
H -2.347421 -1.274881 -3.369930
C -2.565436 1.615239 0.131151
C -3.732133 2.322707 -0.193595
C -4.185134 3.366188 0.615927
C -3.464034 3.708304 1.762117
C -2.295207 3.022299 2.106713
C -1.846262 1.976358 1.293892
O -0.691373 1.274060 1.560126
C 0.204588 1.743147 2.574933
H 0.491338 2.788165 2.385490
H -0.244508 1.642986 3.574638
H 1.100332 1.112788 2.508702
H -1.750221 3.307886 3.005715
H -3.811024 4.520337 2.405468
H -5.096739 3.906999 0.353988
H -4.296525 2.043673 -1.086559
C -1.068690 1.052665 -2.364701
C 0.363280 0.541291 -2.596459
P 1.344003 0.471340 -1.007540
C 1.906081 2.211762 -0.759463
C 0.961972 3.193757 -0.406976
C 1.351362 4.519658 -0.201109
C 2.694796 4.884187 -0.330984
C 3.641476 3.915460 -0.677073
C 3.252724 2.590108 -0.892485
H 4.006861 1.852401 -1.171980
H 4.693205 4.192273 -0.785700
H 3.002604 5.919489 -0.165175
H 0.599864 5.266774 0.066487
H -0.088388 2.933337 -0.285843
C 2.862831 -0.459402 -1.401880
C 3.173706 -0.979302 -2.664482
C 4.324949 -1.749455 -2.858490
C 5.178204 -1.996510 -1.782401
C 4.895406 -1.482323 -0.511927
C 3.737221 -0.720783 -0.318537
O 3.365926 -0.184314 0.874585
C 4.260255 -0.222334 1.974958
H 3.765220 0.313475 2.795816
H 5.210592 0.285131 1.736311
H 4.470744 -1.255397 2.300662
H 5.575270 -1.683535 0.315563
H 6.081449 -2.594402 -1.925970
H 4.553646 -2.148586 -3.848742
H 2.519738 -0.783819 -3.515858
H 0.337324 -0.488656 -2.983124
H 0.877127 1.168799 -3.340720
H -1.687792 0.906111 -3.262193
H -1.068540 2.133590 -2.162357

^{4}10B-07
Geometry with 85 atoms:
Total energy: -3274.528577540
Cr -0.011917 0.063570 0.990549
C 1.264843 0.621578 2.498424
C 0.766313 0.164860 3.875058
C -0.636349 0.676859 4.234512
C -1.795856 0.248264 3.318169
C -2.396160 -1.147164 3.530277
H -2.732965 -1.188356 4.581229
H -3.315050 -1.217460 2.920568
C -1.545733 -2.395286 3.247251
C -1.179782 -2.666781 1.776396
C 0.062127 -1.971376 1.209073
H 0.946576 -2.149700 1.843335
H 0.293347 -2.381605 0.210046
H -1.015382 -3.757882 1.681234
H -2.062979 -2.464613 1.143305
H -2.136988 -3.254435 3.606419
H -0.632289 -2.392183 3.864956
H -1.554839 0.399316 2.234205
H -2.616931 0.975684 3.436842
H -0.602699 1.780237 4.252666
H -0.895643 0.371635 5.263434
H 1.460811 0.508026 4.667086
H 0.788011 -0.935054 3.931786
H 2.255633 0.200820 2.277766
H 1.384745 1.721970 2.467311
P 1.646142 0.173186 -0.861094
C 2.906999 1.490692 -0.735160
C 2.476250 2.765773 -0.328259
C 3.392325 3.811035 -0.202784
C 4.747980 3.587960 -0.469033
C 5.181113 2.319636 -0.866157
C 4.266298 1.270860 -1.001506
H 4.615873 0.285179 -1.315855
H 6.239261 2.142862 -1.074241
H 5.467359 4.403860 -0.364514
H 3.049727 4.800479 0.110387
H 1.420447 2.939469 -0.106041
C 2.506322 -1.375713 -1.314593
C 2.435539 -1.943991 -2.595424
C 3.052301 -3.165442 -2.878638
C 3.752359 -3.830654 -1.870595
C 3.853017 -3.281651 -0.589805
C 3.238622 -2.052855 -0.307950
O 3.308676 -1.429464 0.885810
C 3.932321 -2.066430 1.990509
H 3.451842 -3.032175 2.221764
H 5.009527 -2.223313 1.809607
H 3.809044 -1.389869 2.845886
H 4.414310 -3.808474 0.181154
H 4.236175 -4.788091 -2.079205
H 2.985571 -3.590534 -3.882060
H 1.897501 -1.434540 -3.395775
C 0.654517 0.631121 -2.371617
C -0.612086 -0.225350 -2.509721
P -1.650784 -0.059607 -0.974592
C -3.041513 -1.232128 -1.137708
C -4.241777 -0.961740 -0.453997
C -5.274887 -1.900242 -0.445268
C -5.122305 -3.121301 -1.111556
C -3.931927 -3.397483 -1.789078
C -2.893356 -2.461414 -1.801729
H -1.969229 -2.707157 -2.328687
H -3.806102 -4.348668 -2.312014
H -5.931227 -3.855767 -1.102482
H -6.203917 -1.676620 0.084937
H -4.373330 -0.011336 0.070071
C -2.386713 1.605886 -1.175404
C -3.333288 1.866409 -2.179620
C -3.879217 3.138378 -2.346390
C -3.471779 4.169133 -1.496576
C -2.530733 3.938123 -0.490254
C -1.981341 2.657634 -0.326573
O -1.039460 2.378928 0.645556
C -0.782583 3.393304 1.625979
H -1.705975 3.652267 2.167729
H -0.356886 4.295602 1.160760
H -0.053859 2.975735 2.324588
H -2.234046 4.763503 0.154166
H -3.889136 5.172463 -1.610789
H -4.617058 3.322596 -3.129868
H -3.656186 1.050164 -2.831059
H -1.199205 0.073636 -3.392576
H -0.353303 -1.288337 -2.627331
H 0.396375 1.694486 -2.237894
H 1.283815 0.578043 -3.273178

^{4}10B-08
Geometry with 85 atoms:
Total energy: -3274.530291920
Cr 0.241641 -0.350657 1.079480
C 0.279005 1.444389 2.054227
C -0.988989 1.676515 2.880595
C -1.214270 0.564740 3.911902
C -1.668831 -0.759256 3.289522
C -1.367852 -2.020967 4.095933
H -1.848184 -1.914087 5.084658
H -1.863144 -2.881048 3.610071
C 0.118639 -2.355384 4.295650
C 0.932872 -2.651129 3.020859
C 1.534121 -1.446466 2.271622
H 2.044357 -0.779666 2.989317
H 2.310399 -1.814543 1.575349
H 1.766099 -3.316439 3.316979
H 0.316253 -3.272057 2.343227
H 0.159630 -3.244544 4.946800
H 0.617367 -1.552110 4.865196
H -1.239245 -0.911502 2.263788
H -2.747310 -0.703737 3.065124
H -1.972535 0.865859 4.654159
H -0.277086 0.415515 4.472454
H -1.873701 1.757882 2.220551
H -0.923921 2.648615 3.406111
H 1.173001 1.444991 2.701448
H 0.407289 2.226846 1.294004
P -1.507185 0.345276 -0.830625
C -2.683277 -1.024200 -1.175609
C -2.836770 -1.634352 -2.430418
C -3.711128 -2.715379 -2.588537
C -4.450627 -3.191080 -1.502056
C -4.319489 -2.577196 -0.251369
C -3.439420 -1.505610 -0.089769
H -3.339987 -1.035590 0.891517
H -4.900711 -2.936452 0.601444
H -5.133117 -4.034688 -1.630312
H -3.819274 -3.182352 -3.570681
H -2.282756 -1.274372 -3.299210
C -2.588461 1.840409 -0.861955
C -3.982170 1.746632 -0.998333
C -4.798312 2.878902 -0.922024
C -4.220984 4.129267 -0.703712
C -2.834840 4.256001 -0.573984
C -2.017758 3.120870 -0.659521

O	-0.663538	3.168799	-0.572779
C	-0.014212	4.391899	-0.256228
H	-0.350142	4.785533	0.717867
H	1.059288	4.167955	-0.197458
H	-0.179718	5.151734	-1.039114
H	-2.398266	5.240902	-0.411183
H	-4.847484	5.022085	-0.636443
H	-5.880003	2.777624	-1.032134
H	-4.445590	0.773224	-1.163366
C	-0.420868	0.423361	-2.354187
C	0.950503	1.061830	-2.099004
P	1.818630	0.277509	-0.656809
C	3.280738	1.302826	-0.304905
C	3.945800	1.103050	0.918395
C	5.068056	1.868519	1.238593
C	5.530291	2.844065	0.348503
C	4.869482	3.051196	-0.865803
C	3.748274	2.283702	-1.196494
H	3.249060	2.456876	-2.151657
H	5.229138	3.811517	-1.563349
H	6.406407	3.445441	0.603227
H	5.579815	1.706648	2.190241
H	3.582249	0.351134	1.621180
C	2.415725	-1.317665	-1.324873
C	3.636968	-1.448371	-1.999084
C	4.038340	-2.682148	-2.515991
C	3.207619	-3.792607	-2.358004
C	1.987053	-3.688151	-1.681963
C	1.592119	-2.452248	-1.157313
O	0.412902	-2.271147	-0.463369
C	-0.460844	-3.396230	-0.305055
H	-0.837228	-3.734226	-1.282515
H	-1.306972	-3.055406	0.299192
H	0.049982	-4.221574	0.212894
H	1.365343	-4.574830	-1.569450
H	3.508128	-4.763299	-2.759562
H	4.993703	-2.774409	-3.036511
H	4.283359	-0.574274	-2.112208
H	1.587475	0.957954	-2.991370
H	0.843362	2.127929	-1.866249
H	-0.284914	-0.621634	-2.673464
H	-0.945390	0.950962	-3.165041

^{4}10B-09

Geometry with 85 atoms:

Total energy: -3274.529760670

Cr	-0.443942	-0.884899	0.867659
C	0.639234	-1.643229	2.466240
C	-0.245077	-1.845482	3.710749
C	-1.526457	-2.626742	3.403789
C	-2.567606	-1.811264	2.628994
C	-3.643865	-2.617926	1.901158
H	-4.218105	-3.174547	2.662882
H	-4.357604	-1.917907	1.432164
C	-3.147372	-3.607997	0.837108
C	-2.398119	-3.011711	-0.366290
C	-0.927719	-2.619191	-0.151958
H	-0.397035	-3.433983	0.371772
H	-0.429091	-2.502000	-1.132113
H	-2.424177	-3.775903	-1.166715
H	-2.982834	-2.165697	-0.767201
H	-4.035256	-4.139999	0.455956
H	-2.518247	-4.385803	1.304439
H	-2.106924	-1.119884	1.874223
H	-3.039918	-1.082599	3.310012
H	-2.003720	-2.975514	4.335487
H	-1.258158	-3.534239	2.839315
H	-0.523670	-0.872667	4.159337
H	0.321596	-2.376616	4.499020
H	1.055682	-2.615924	2.149639
H	1.505488	-0.999052	2.701226
P	-1.605111	0.503761	-0.912590
C	-3.321371	0.359393	-1.518173
C	-3.638295	-0.074854	-2.815127
C	-4.975190	-0.254464	-3.186808
C	-6.001362	-0.002169	-2.273384
C	-5.691060	0.434607	-0.979775
C	-4.359944	0.610209	-0.601805
H	-4.125506	0.946248	0.412536
H	-6.490107	0.635209	-0.261974
H	-7.043917	-0.145013	-2.567532
H	-5.212468	-0.593003	-4.198318
H	-2.854117	-0.281778	-3.545609
C	-1.451137	2.236768	-0.345415
C	-1.925990	3.307104	-1.120323
C	-1.821675	4.623323	-0.673045
C	-1.243825	4.871883	0.574661
C	-0.767406	3.825026	1.367380
C	-0.861761	2.502061	0.910068
O	-0.386063	1.432630	1.642945
C	0.245092	1.715671	2.903824
H	1.090273	2.404874	2.768704
H	-0.485690	2.135200	3.612886
H	0.623979	0.765622	3.283700
H	-0.322756	4.054930	2.333310
H	-1.161684	5.896038	0.946605
H	-2.195381	5.445871	-1.286181
H	-2.397554	3.097281	-2.084162
C	-0.501511	0.373660	-2.397130
C	0.956371	0.676568	-2.030270
P	1.543792	-0.194405	-0.477586
C	2.572108	1.019547	0.446978
C	3.482774	0.513631	1.391552
C	4.238875	1.381988	2.181796
C	4.096023	2.766699	2.041110
C	3.192444	3.275616	1.104062
C	2.431767	2.408827	0.313118
H	1.726593	2.838712	-0.398549
H	3.072993	4.355363	0.984443
H	4.689789	3.445853	2.657735
H	4.945260	0.973580	2.908658
H	3.610198	-0.565315	1.506187
C	2.739830	-1.466891	-1.009010
C	2.596168	-2.803768	-0.613649
C	3.546493	-3.764382	-0.970289
C	4.656137	-3.381797	-1.725611
C	4.828338	-2.053381	-2.127570
C	3.874294	-1.089418	-1.773939
O	3.955483	0.216649	-2.112012
C	5.118079	0.720205	-2.751829
H	4.965939	1.802960	-2.853879
H	5.254605	0.279353	-3.754319
H	6.021729	0.539479	-2.145018
H	5.704245	-1.776452	-2.714054
H	5.407482	-4.123118	-2.009088
H	3.420530	-4.801655	-0.653938
H	1.736176	-3.095774	-0.012818
H	1.632898	0.402090	-2.849780
H	1.083528	1.755685	-1.870635
H	-0.609280	-0.658342	-2.768873
H	-0.840463	1.052738	-3.195237

^{4}10B-10

Geometry with 85 atoms:

Total energy: -3274.527805210

Cr	-0.384249	-0.641386	0.860414
C	-1.815040	-1.154195	2.248234
C	-1.240287	-1.922426	3.447110
C	0.086837	-1.358328	3.969306
C	1.289127	-1.533095	3.028893
C	1.745404	-2.995558	2.809718
H	2.782956	-3.091191	3.169932
H	1.145980	-3.655119	3.459813
C	1.689055	-3.544509	1.374910
C	0.288769	-3.691803	0.747028
C	-0.250939	-2.489482	-0.040103
H	0.377501	-2.335834	-0.938466
H	-1.270605	-2.726761	-0.392845
H	0.328419	-4.550925	0.050372
H	-0.431776	-3.995203	1.525800
H	2.168941	-4.537178	1.395814
H	2.315666	-2.921037	0.716807
H	2.129873	-0.936786	3.419989
H	1.156639	-1.061027	2.021166
H	0.353639	-1.846193	4.923004
H	-0.045139	-0.288359	4.209523
H	-1.100699	-2.982775	3.180922
H	-1.966734	-1.926114	4.282251
H	-2.232685	-0.183838	2.583330
H	-2.634294	-1.721570	1.776762
P	1.253023	0.539715	-0.906396
C	2.280762	2.008028	-0.488010
C	2.563600	3.017105	-1.423939
C	3.331794	4.125710	-1.056713
C	3.831855	4.236132	0.244331
C	3.562481	3.231929	1.179833
C	2.790008	2.126569	0.815447
H	2.588627	1.341439	1.545276
H	3.955371	3.310046	2.196843
H	4.433917	5.102949	0.527936
H	3.543938	4.904705	-1.793194
H	2.193286	2.946349	-2.448885
C	2.379535	-0.606749	-1.790316
C	2.211636	-1.008732	-3.121254
C	3.075931	-1.940502	-3.706082
C	4.121795	-2.475923	-2.953653
C	4.306577	-2.098909	-1.619240
C	3.431390	-1.176137	-1.034558
O	3.501130	-0.774268	0.261192
C	4.605420	-1.152552	1.065533
H	5.557262	-0.812134	0.623626
H	4.467151	-0.657920	2.036118
H	4.643248	-2.243722	1.222007
H	5.124237	-2.532249	-1.043509
H	4.805846	-3.200158	-3.402590
H	2.931677	-2.240737	-4.746043
H	1.399916	-0.595516	-3.722767
C	0.102059	1.187052	-2.226595
C	-1.148881	0.315630	-2.397499
P	-1.990826	0.106193	-0.757436
C	-3.535974	-0.808185	-1.039133
C	-3.634061	-1.756165	-2.072100
C	-4.795935	-2.520715	-2.211158
C	-5.861009	-2.350454	-1.322225
C	-5.764325	-1.412583	-0.288455
C	-4.606892	-0.646471	-0.141384
H	-4.538105	0.080297	0.671121
H	-6.593528	-1.278243	0.410242
H	-6.767874	-2.949609	-1.433879
H	-4.866820	-3.252871	-3.019127
H	-2.810947	-1.907196	-2.773334
C	-2.444688	1.800080	-0.250765
C	-3.452135	2.526217	-0.904226
C	-3.761219	3.830090	-0.516762
C	-3.054138	4.414951	0.536957
C	-2.046622	3.713257	1.204622
C	-1.737556	2.404576	0.811568
O	-0.748514	1.661754	1.416508
C	-0.112609	2.178535	2.589769
H	0.601072	1.414597	2.917753
H	-0.850888	2.352561	3.388503
H	0.437862	3.104102	2.364989
H	-1.513447	4.196195	2.022073
H	-3.286224	5.435093	0.852035
H	-4.549954	4.383875	-1.029894
H	-4.008039	2.053934	-1.718320
H	-1.849112	0.761592	-3.121724
H	-0.888360	-0.692780	-2.756725
H	-0.185220	2.197344	-1.894523
H	0.625199	1.308370	-3.186723

^{4}10B-11

Geometry with 85 atoms:

Total energy: -3274.528079880

Cr	0.224234	-0.128862	1.095262
C	-0.188304	1.717543	1.846211
C	-1.451024	1.680237	2.709189
C	-1.413979	0.570999	3.770409
C	-1.631792	-0.826556	3.179776
C	-1.137300	-2.011502	4.008381
H	-1.675714	-2.000004	4.972457
H	-1.446767	-2.944057	3.502748
C	0.373453	-2.078799	4.285671
C	1.303955	-2.120782	3.057393
C	1.662408	-0.765007	2.420289
H	1.847985	-0.007420	3.201515
H	2.597275	-0.860327	1.841450
H	2.239993	-2.619063	3.373113
H	0.872493	-2.812855	2.303726
H	0.544447	-2.988804	4.884741
H	0.678167	-1.239132	4.934033
H	-1.198072	-0.928827	2.149521
H	-2.703163	-0.954063	2.947619

H	-2.192199	0.736608	4.534190
H	-0.448583	0.616831	4.300209
H	-2.342533	1.546343	2.069638
H	-1.586712	2.657529	3.210899
H	0.694886	2.016197	2.434951
H	-0.292762	2.406087	0.996492
P	-1.505184	-0.155386	-0.882310
C	-1.670214	-1.934246	-1.315129
C	-2.126532	-2.799776	-0.300461
C	-2.257069	-4.169940	-0.537847
C	-1.908690	-4.699169	-1.785721
C	-1.441750	-3.850609	-2.793652
C	-1.329233	-2.475091	-2.564910
H	-0.976641	-1.833467	-3.374761
H	-1.170426	-4.258959	-3.770329
H	-2.001922	-5.771756	-1.972062
H	-2.625341	-4.825956	0.254607
H	-2.398647	-2.397244	0.679287
C	-3.216966	0.503763	-0.935583
C	-4.338350	-0.298416	-1.189499
C	-5.629538	0.235929	-1.146924
C	-5.805431	1.587114	-0.846222
C	-4.703849	2.412238	-0.597828
C	-3.409783	1.877465	-0.645862
O	-2.281168	2.602330	-0.440471
C	-2.369329	3.973323	-0.082225
H	-2.922462	4.109588	0.862254
H	-1.338222	4.325211	0.052561
H	-2.850024	4.566799	-0.878713
H	-4.861121	3.466471	-0.371183
H	-6.810431	2.014349	-0.806279
H	-6.491023	-0.403832	-1.349256
H	-4.205818	-1.356478	-1.422304
C	-0.646854	0.659780	-2.317055
C	0.850630	0.341220	-2.346825
P	1.696539	0.631835	-0.716087
C	2.158799	2.390641	-0.613336
C	1.747341	3.342518	-1.559402
C	2.053502	4.694675	-1.371011
C	2.772374	5.103348	-0.244417
C	3.183543	4.157872	0.702449
C	2.870288	2.809979	0.526471
H	3.179549	2.079037	1.278105
H	3.743246	4.473197	1.586291
H	3.011988	6.159907	-0.101730
H	1.730241	5.429794	-2.112011
H	1.184218	3.044538	-2.445783
C	3.228816	-0.344153	-0.853505
C	4.505076	0.193701	-1.052665
C	5.622767	-0.644185	-1.117558
C	5.458318	-2.024004	-0.983124
C	4.190272	-2.583448	-0.785569
C	3.073629	-1.743682	-0.719359
O	1.792992	-2.175177	-0.531018
C	1.529349	-3.571258	-0.436596
H	1.822135	-4.092238	-1.363043
H	0.447860	-3.672305	-0.296362
H	2.053412	-4.019869	0.422689
H	4.086964	-3.663186	-0.682356
H	6.327155	-2.685119	-1.030491
H	6.616191	-0.218218	-1.272146
H	4.627306	1.274125	-1.154146
H	1.020649	-0.727165	-2.545293
H	1.373894	0.901232	-3.137530
H	-1.137163	0.380012	-3.262535
H	-0.822036	1.734915	-2.166911

[4]10B-12
Geometry with 85 atoms:
Total energy: -3274.525426680

Cr	-0.320927	0.028980	1.142258
C	-1.768801	0.662510	2.478969
C	-1.413785	0.820551	3.967436
C	-0.221343	1.753254	4.284170
C	1.165688	1.104973	4.461936
C	1.592872	0.110358	3.370102
H	1.150571	0.462112	2.400500
H	2.669536	0.205484	3.153606
C	1.274200	-1.365226	3.668317
C	1.065140	-2.242794	2.430034
C	-0.251139	-1.924462	1.714918
H	-0.375874	-2.551939	0.820729
H	-1.113475	-2.100657	2.381182
H	1.922641	-2.131111	1.740436
H	1.078913	-3.304597	2.743738
H	0.370324	-1.429039	4.293835
H	2.096633	-1.759035	4.289065
H	1.201845	0.576858	5.430701
H	1.910500	1.914905	4.537004
H	-0.433338	2.315223	5.208734
H	-0.160063	2.519560	3.490134
H	-1.249286	-0.167136	4.429736
H	-2.301952	1.226534	4.487649
H	-2.109802	1.638138	2.078589
H	-2.614921	-0.039495	2.377744
P	-1.820674	-0.304402	-0.720081
C	-3.365906	-1.252578	-0.563497
C	-3.496008	-2.544853	-1.100085
C	-4.671063	-3.273607	-0.893510
C	-5.719837	-2.722703	-0.152407
C	-5.594270	-1.436648	0.384802
C	-4.423575	-0.703796	0.185387
H	-4.335855	0.300094	0.606736
H	-6.412273	-1.001396	0.963712
H	-6.637120	-3.294742	0.006422
H	-4.766043	-4.276160	-1.317589
H	-2.690867	-2.993287	-1.684907
C	-2.273254	1.379158	-1.272118
C	-3.318496	1.615422	-2.177540
C	-3.613156	2.909311	-2.609067
C	-2.849981	3.978670	-2.134594
C	-1.803598	3.770012	-1.231519
C	-1.514579	2.470494	-0.795906
O	-0.498150	2.193013	0.091189
C	0.189898	3.287816	0.708175
H	0.900657	2.850520	1.415471
H	0.750929	3.866733	-0.039661
H	-0.516653	3.934281	1.250982
H	-1.226012	4.622857	-0.878434
H	-3.068306	4.996948	-2.465163
H	-4.433032	3.081170	-3.309352
H	-3.916237	0.773986	-2.536884
C	-0.885155	-1.012815	-2.155576
C	0.427325	-0.250971	-2.382186
P	1.491279	-0.153835	-0.839177
C	2.390064	1.448981	-0.953686
C	2.334075	2.323846	-2.049439
C	2.997646	3.555536	-2.006690
C	3.737170	3.922468	-0.879019
C	3.813338	3.050238	0.212540
C	3.138748	1.829084	0.177047
H	3.197831	1.159479	1.039541
H	4.393837	3.324948	1.096778
H	4.257166	4.883089	-0.851929
H	2.941464	4.227538	-2.866719
H	1.777700	2.060455	-2.950415
C	2.833882	-1.396960	-1.077753
C	4.184386	-1.038577	-1.205332
C	5.186157	-2.008166	-1.308475
C	4.841263	-3.359117	-1.285944
C	3.502765	-3.746750	-1.172889
C	2.500237	-2.772867	-1.074514
O	1.177165	-3.065820	-0.985806
C	0.759498	-4.415789	-0.853314
H	1.201090	-4.889038	0.039690
H	1.014623	-5.008434	-1.748531
H	-0.332340	-4.395534	-0.737804
H	3.249536	-4.806441	-1.165989
H	5.615065	-4.127035	-1.361527
H	6.229952	-1.702542	-1.406360
H	4.467042	0.014423	-1.224404
H	1.004271	-0.708757	-3.199026
H	0.199247	0.783203	-2.681045
H	-0.677373	-2.065378	-1.924325
H	-1.521956	-0.970306	-3.053695

[4]10B-13
Geometry with 85 atoms:
Total energy: -3274.527040970

Cr	0.073643	-0.500473	1.044365
C	1.278324	-1.694581	2.223112
C	0.561746	-2.371994	3.402543
C	-0.807685	-2.964710	3.051856
C	-1.898229	-1.932246	2.738050
C	-2.328172	-1.034074	3.920152
H	-3.400346	-1.201544	4.113595
H	-1.808009	-1.370542	4.832998
C	-2.104445	0.479333	3.765590
C	-0.637493	0.957277	3.700201
C	-0.038239	1.111331	2.301373
H	-0.628004	1.845345	1.729618
H	0.995917	1.492848	2.359487
H	-0.591779	1.950402	4.187466
H	-0.008781	0.306617	4.330689
H	-2.593491	0.963408	4.626950
H	-2.648355	0.848837	2.875098
H	-2.774383	-2.451497	2.318372
H	-1.613409	-1.269523	1.878450
H	-1.174527	-3.584685	3.888589
H	-0.696953	-3.651352	2.194259
H	0.443211	-1.659640	4.235187
H	1.196377	-3.183495	3.807008
H	1.652647	-2.468343	1.526126
H	2.162803	-1.144420	2.587518
P	-1.406583	0.470982	-0.930587
C	-2.890330	-0.542418	-1.300065
C	-3.165286	-1.107595	-2.555634
C	-4.283814	-1.930288	-2.729013
C	-5.143073	-2.188997	-1.657533
C	-4.886598	-1.616104	-0.406455
C	-3.765528	-0.803624	-0.227969
H	-3.572694	-0.361804	0.753237
H	-5.558904	-1.806394	0.433719
H	-6.015303	-2.832086	-1.797265
H	-4.486091	-2.366649	-3.710336
H	-2.515770	-0.912486	-3.410651
C	-2.032735	2.201113	-0.942541
C	-3.362562	2.512778	-1.265257
C	-3.834727	3.826220	-1.196472
C	-2.971770	4.846928	-0.795927
C	-1.640659	4.567001	-0.473671
C	-1.165331	3.250999	-0.553525
O	0.120380	2.902097	-0.282764
C	0.996174	3.843046	0.322888
H	0.576695	4.229388	1.266504
H	1.928473	3.307404	0.536830
H	1.215280	4.684295	-0.356530
H	-0.979354	5.377204	-0.167296
H	-3.330468	5.877204	-0.732563
H	-4.873636	4.045696	-1.451416
H	-4.045382	1.717026	-1.568066
C	-0.317199	0.308241	-2.437462
C	1.119758	0.780081	-2.179619
P	1.827817	0.061307	-0.608631
C	3.303992	1.055303	-0.220343
C	3.738344	1.111981	1.115396
C	4.855694	1.876842	1.458600
C	5.543752	2.594489	0.474879
C	5.115831	2.542741	-0.855820
C	4.001194	1.776417	-1.206170
H	3.684671	1.745341	-2.250501
H	5.652707	3.100334	-1.627116
H	6.415080	3.196038	0.745218
H	5.185926	1.916176	2.499252
H	3.196901	0.563548	1.888175
C	2.423524	-1.589695	-1.144704
C	3.739284	-1.850220	-1.544934
C	4.118337	-3.131857	-1.955826
C	3.174417	-4.159384	-1.965027
C	1.854742	-3.924786	-1.560886
C	1.484112	-2.642524	-1.147459
O	0.216326	-2.322016	-0.712292
C	-0.804296	-3.323750	-0.749482
H	-0.541699	-4.180583	-0.109708
H	-0.975854	-3.665413	-1.782247
H	-1.719171	-2.850668	-0.375875
H	1.138107	-4.745273	-1.564586
H	3.460651	-5.164721	-2.283086
H	5.148185	-3.324080	-2.263546
H	4.477091	-1.044904	-1.529305
H	1.769183	0.490021	-3.019637
H	1.161435	1.871008	-2.069920
H	-0.320195	-0.761671	-2.694704

H -0.754701 0.860368 -3.283111

^{4}10B-14
Geometry with 85 atoms:
Total energy: -3274.526712090
Cr 0.193943 -0.374524 1.142918
C 1.490348 -1.398547 2.398855
C 0.703759 -2.322754 3.347804
C -0.326944 -1.568576 4.195690
C -1.550138 -1.096770 3.398509
C -2.276244 0.161656 3.919390
H -3.247820 -0.131862 4.348228
H -1.699586 0.603743 4.749541
C -2.500313 1.232411 2.839941
C -1.261729 2.073086 2.471014
C 0.074515 1.350896 2.253177
H 0.814333 2.043038 1.817685
H 0.489639 1.020224 3.220797
H -1.519506 2.662546 1.579828
H -1.115270 2.814658 3.281572
H -3.291677 1.924316 3.172574
H -2.905919 0.748209 1.933815
H -2.256910 -1.935494 3.279887
H -1.290142 -0.900551 2.325512
H 0.167821 -0.698121 4.658763
H -0.679623 -2.196695 5.031139
H 1.404113 -2.852669 4.021091
H 0.190326 -3.122421 2.780521
H 2.202904 -1.987869 1.796419
H 2.082559 -0.681902 2.994524
P 1.851412 0.078314 -0.596347
C 3.271029 1.187746 -0.341392
C 3.728660 1.382186 0.973870
C 4.804357 2.237575 1.222632
C 5.425980 2.908643 0.164613
C 4.972817 2.721594 -1.145468
C 3.899261 1.864561 -1.402247
H 3.559806 1.731067 -2.431512
H 5.457727 3.244649 -1.973258
H 6.264673 3.580997 0.361213
H 5.153942 2.383819 2.247343
H 3.238483 0.868444 1.802956
C 2.508146 -1.587432 -0.990097
C 3.794932 -1.809741 -1.494684
C 4.227979 -3.103678 -1.797623
C 3.364962 -4.181481 -1.595568
C 2.076388 -3.984244 -1.085769
C 1.651382 -2.688484 -0.777868
O 0.406845 -2.405241 -0.254571
C -0.503970 -3.485638 -0.023666
H -0.075289 -4.220205 0.675215
H -1.406625 -3.046548 0.413749
H -0.773174 -3.976467 -0.971754
H 1.425428 -4.843303 -0.929695
H 3.692210 -5.197534 -1.828659
H 5.235291 -3.266306 -2.186295
H 4.467613 -0.961822 -1.643979
C 1.061474 0.591399 -2.200312
C -0.324913 -0.042360 -2.371603
P -1.431476 0.164389 -0.875575
C -2.762136 -1.074282 -1.140650
C -3.010696 -1.693551 -2.377275
C -4.009973 -2.665589 -2.492904
C -4.780542 -3.022235 -1.382539
C -4.550929 -2.401201 -0.150298
C -3.545317 -1.439649 -0.029719
H -3.368684 -0.971043 0.941328
H -5.151986 -2.670264 0.721768
H -5.561617 -3.780565 -1.477582
H -4.190199 -3.141719 -3.459978
H -2.434749 -1.424198 -3.264180
C -2.268890 1.782908 -1.115718
C -3.628612 1.888647 -1.440333
C -4.247226 3.137283 -1.555023
C -3.501115 4.296301 -1.339755
C -2.142608 4.219791 -1.015556
C -1.523562 2.968377 -0.907122
O -0.210891 2.800595 -0.596894
C 0.587436 3.920546 -0.245347
H 1.584635 3.528875 -0.007351
H 0.182526 4.440519 0.638775
H 0.674103 4.633569 -1.083039
H -1.576846 5.135545 -0.845871
H -3.974389 5.277710 -1.423137
H -5.307530 3.199082 -1.808755
H -4.216480 0.982996 -1.600672
H -0.822577 0.370066 -3.262194
H -0.226062 -1.129183 -2.517502
H 0.997368 1.686243 -2.192784
H 1.720456 0.285253 -3.027276

^{4}10B-15
Geometry with 85 atoms:
Total energy: -3274.529060300
Cr -0.101232 0.020083 1.246081
C -1.694591 0.159538 2.559262
C -2.347560 -1.176836 2.913246
C -1.310890 -2.251754 3.252360
C -0.533493 -2.726813 2.024289
C 0.751890 -3.506728 2.288089
H 0.485439 -4.424487 2.841908
H 1.166212 -3.840588 1.320616
C 1.848956 -2.761255 3.060783
C 2.402570 -1.486015 2.402548
C 1.541205 -0.215492 2.502863
H 1.149004 -0.097734 3.530696
H 2.186590 0.657620 2.310942
H 3.378403 -1.279955 2.883052
H 2.647893 -1.710451 1.346867
H 2.684078 -3.468698 3.197912
H 1.498579 -2.518588 4.079136
H -0.264479 -1.899219 1.313946
H -1.209277 -3.319888 1.387722
H -1.794615 -3.135312 3.703131
H -0.622060 -1.855920 4.016038
H -2.973791 -1.527388 2.072116
H -3.039584 -1.054318 3.768329
H -1.200189 0.601137 3.446156
H -2.439846 0.894015 2.207880
P 1.505878 0.259607 -0.828898
C 2.777353 1.554604 -0.553459
C 2.645875 2.863332 -1.048855
C 3.562685 3.856589 -0.687841
C 4.623227 3.560121 0.171748
C 4.764877 2.260410 0.669798
C 3.849327 1.268151 0.316003
H 3.974669 0.260507 0.716279
H 5.592234 2.015862 1.340393
H 5.339188 4.336990 0.450423
H 3.446806 4.866626 -1.088853
H 1.830335 3.130614 -1.721876
C 2.407920 -1.214875 -1.453896
C 3.742769 -1.179530 -1.882326
C 4.392681 -2.338092 -2.316751
C 3.702412 -3.550574 -2.328467
C 2.366034 -3.612324 -1.921789
C 1.716321 -2.449414 -1.488780
O 0.411874 -2.422921 -1.092473
C -0.403702 -3.569458 -1.285940
H -0.424379 -3.868997 -2.348056
H -0.063556 -4.422201 -0.675838
H -1.416161 -3.287604 -0.971707
H 1.840147 -4.566266 -1.943306
H 4.201268 -4.463984 -2.661525
H 5.432651 -2.288887 -2.645944
H 4.286823 -0.233668 -1.876954
C 0.507702 0.840738 -2.301639
C -0.858666 0.151504 -2.373696
P -1.692613 0.263650 -0.713602
C -3.336417 -0.504040 -0.909920
C -3.550020 -1.540733 -1.835890
C -4.787017 -2.190862 -1.891661
C -5.820132 -1.815648 -1.028610
C -5.614181 -0.784095 -0.105924
C -4.380793 -0.133717 -0.042250
H -4.231484 0.671051 0.680715
H -6.418621 -0.483366 0.569604
H -6.785987 -2.324214 -1.076171
H -4.943273 -2.991651 -2.618758
H -2.759067 -1.849358 -2.521928
C -1.993423 2.067848 -0.551592
C -2.988975 2.712489 -1.303082
C -3.198562 4.087545 -1.202011
C -2.398969 4.835053 -0.335934
C -1.399472 4.221669 0.423854
C -1.193373 2.839892 0.319366
O -0.196347 2.199830 1.050273
C 0.590209 3.001098 1.956632
H 1.139451 3.772556 1.398743
H 1.305503 2.328545 2.434279
H -0.057345 3.452999 2.722217
H -0.796032 4.833680 1.090817
H -2.549567 5.912915 -0.240237
H -3.980624 4.569721 -1.791990
H -3.617754 2.116868 -1.969572
H -1.494610 0.616582 -3.143384
H -0.745768 -0.913032 -2.617188
H 0.360214 1.924957 -2.186464
H 1.086294 0.682443 -3.224180

^{4}10B-16
Geometry with 85 atoms:
Total energy: -3274.526662600
Cr 0.203051 -0.371704 1.140472
C 1.525369 -1.380574 2.380868
C 0.760535 -2.311645 3.340753
C -0.271117 -1.568049 4.196867
C -1.509387 -1.113143 3.412843
C -2.244122 0.137572 3.940616
H -3.208822 -0.166273 4.377692
H -1.664974 0.585220 4.766038
C -2.489279 1.206786 2.864176
C -1.263372 2.060456 2.482914
C 0.078287 1.352859 2.250996
H 0.805707 2.053234 1.807627
H 0.507924 1.027704 3.214050
H -1.536752 2.646372 1.594093
H -1.116796 2.803927 3.291714
H -3.284302 1.890369 3.205288
H -2.899313 0.719214 1.961755
H -2.207308 -1.960779 3.305847
H -1.266944 -0.916749 2.335699
H 0.217603 -0.690609 4.653035
H -0.606990 -2.198503 5.037489
H 1.474093 -2.830104 4.009166
H 0.252065 -3.119980 2.781398
H 2.238857 -1.962869 1.772574
H 2.112177 -0.651731 2.966823
P 1.840069 0.113876 -0.608042
C 3.272758 1.204826 -0.346123
C 3.897333 1.180297 0.914303
C 4.989850 2.010437 1.170908
C 5.463063 2.875952 0.178602
C 4.844291 2.906399 -1.074680
C 3.752899 2.074043 -1.340863
H 3.285360 2.111911 -2.326357
H 5.212865 3.579778 -1.852344
H 6.315129 3.528727 0.383333
H 5.469615 1.985440 2.152125
H 3.526557 0.514012 1.695970
C 2.496641 -1.544862 -1.029048
C 3.773965 -1.747770 -1.565175
C 4.213384 -3.033547 -1.891767
C 3.365854 -4.122275 -1.681546
C 2.086837 -3.944137 -1.141646
C 1.655177 -2.655994 -0.810748
O 0.418458 -2.390466 -0.260628
C -0.473176 -3.483785 -0.014647
H -0.020271 -4.214177 0.673182
H -1.372589 -3.058072 0.442213
H -0.754925 -3.975308 -0.958640
H 1.448284 -4.811639 -0.981220
H 3.698193 -5.132390 -1.932608
H 5.213057 -3.181890 -2.305157
H 4.432642 -0.889646 -1.720407
C 1.036764 0.641662 -2.198633
C -0.337833 -0.018292 -2.369499
P -1.439401 0.162042 -0.866171
C -2.748802 -1.100522 -1.123552
C -2.987244 -1.732059 -2.355748
C -3.968524 -2.723273 -2.463838
C -4.730897 -3.087141 -1.350187
C -4.511379 -2.454001 -0.122200

C -3.523737 -1.473185 -0.009158
H -3.354309 -0.995581 0.958730
H -5.106118 -2.728685 0.752451
H -5.497638 -3.860676 -1.439234
H -4.141099 -3.208850 -3.427600
H -2.417213 -1.457507 -3.244906
C -2.308923 1.765298 -1.098369
C -3.672301 1.845198 -1.415048
C -4.315715 3.081743 -1.524275
C -3.591012 4.254780 -1.311817
C -2.229301 4.204211 -0.996103
C -1.585561 2.964893 -0.892990
O -0.267548 2.822444 -0.592434
C 0.510194 3.956245 -0.239309
H 1.516497 3.583213 -0.009570
H 0.099962 4.463612 0.649694
H 0.577926 4.675173 -1.073759
H -1.679954 5.130495 -0.829451
H -4.083884 5.226839 -1.390991
H -5.378540 3.123204 -1.771516
H -4.243616 0.928654 -1.573042
H -0.846811 0.389848 -3.255577
H -0.218240 -1.101967 -2.522803
H 0.944401 1.733735 -2.174578
H 1.698835 0.363215 -3.033121

^{4}10B-17(10')
Geometry with 85 atoms:
Total energy: -3274.525949460
Cr -0.042948 -0.176020 0.977062
C 0.986480 -0.036706 2.724122
C -0.377287 0.148534 3.348939
C -0.773216 -0.809899 4.485225
C -0.891042 -2.265950 4.028306
C -2.143906 -2.549836 3.174347
H -2.957115 -2.876284 3.843709
H -2.515673 -1.616632 2.712708
C -1.929587 -3.586931 2.061116
C -1.476388 -3.012129 0.710519
C -0.156729 -2.227026 0.655457
H 0.617982 -2.682004 1.295086
H 0.232513 -2.272188 -0.376109
H -1.399675 -3.863694 0.006753
H -2.301518 -2.398981 0.309217
H -2.871884 -4.133002 1.884415
H -1.205071 -4.347177 2.407133
H -0.895487 -2.928575 4.909306
H 0.016574 -2.537608 3.467141
H -1.730175 -0.481989 4.928163
H -0.011244 -0.716388 5.276672
H -1.206014 0.010192 2.555218
H -0.542302 1.196440 3.647007
H 1.486126 -0.980684 2.979821
H 1.670404 0.808305 2.867825
P 1.632383 0.278665 -0.821416
C 3.040601 1.389909 -0.425748
C 3.400273 2.469242 -1.250407
C 4.458234 3.309189 -0.888872
C 5.170897 3.076602 0.290781
C 4.823880 1.997641 1.110706
C 3.762994 1.160510 0.759231
H 3.490438 0.323563 1.400975
H 5.379550 1.808337 2.032533
H 5.998008 3.734038 0.569700
H 4.728282 4.146679 -1.536932
H 2.867921 2.666812 -2.182424
C 2.342899 -1.181455 -1.673744
C 2.248962 -1.402891 -3.054150
C 2.753215 -2.572712 -3.630267
C 3.358492 -3.533019 -2.817975
C 3.469979 -3.335433 -1.438549
C 2.968565 -2.160168 -0.863799
O 3.033680 -1.870959 0.455608
C 3.537360 -2.825980 1.374207
H 2.956404 -3.763305 1.340612
H 4.602313 -3.045628 1.185551
H 3.436798 -2.379024 2.371998
H 3.948268 -4.095032 -0.820665
H 3.754270 -4.451559 -3.258198
H 2.672093 -2.729676 -4.707771
H 1.777015 -0.661909 -3.701710
C 0.659065 1.182118 -2.124918
C -0.696456 0.517662 -2.408495
P -1.713877 0.399400 -0.854001
C -3.265470 -0.447919 -1.304018
C -3.471385 -1.060750 -2.549520
C -4.658772 -1.757084 -2.801505
C -5.647533 -1.843794 -1.819243
C -5.449322 -1.232131 -0.575403
C -4.264249 -0.544897 -0.316001
H -4.115036 -0.078851 0.662308
H -6.218880 -1.297055 0.197580
H -6.573187 -2.388391 -2.020505
H -4.808907 -2.231510 -3.774363
H -2.716138 -1.005119 -3.334940
C -2.203696 2.135753 -0.513057
C -3.346899 2.721935 -1.076264
C -3.703295 4.037644 -0.774633
C -2.910274 4.776764 0.104562
C -1.764053 4.216837 0.677789
C -1.408028 2.898494 0.368611
O -0.281782 2.290633 0.893965
C 0.688306 3.128953 1.539572
H 1.576947 2.515567 1.706148
H 0.308586 3.501081 2.503740
H 0.958368 3.974914 0.889374
H -1.166821 4.815083 1.364156
H -3.180504 5.805093 0.356300
H -4.596643 4.479542 -1.220694
H -3.970700 2.133066 -1.752702
H -1.250135 1.079695 -3.177012
H -0.555425 -0.510913 -2.777277
H 0.513621 2.200362 -1.731487
H 1.238352 1.284048 -3.054702

^{4}10B-18
Geometry with 85 atoms:
Total energy: -3274.524989060
Cr -0.078263 -0.061822 1.105037
C -0.911794 1.216679 2.454337
C 0.417126 1.945114 2.633645
C 1.154957 1.813647 3.979592
C 1.819619 0.457601 4.262271
C 0.879738 -0.705052 4.666725
H 0.983201 -0.896305 5.746762
H -0.171956 -0.416900 4.525888
C 1.140930 -2.013179 3.910041
C 0.772826 -1.964571 2.418866
C -0.681794 -1.741630 2.068561
H -1.106810 -2.486170 1.386700
H -1.342822 -1.587536 2.930949
H 1.417704 -1.130231 1.966187
H 1.185623 -2.839776 1.890905
H 0.563682 -2.831605 4.371972
H 2.206104 -2.286860 4.010960
H 2.569546 0.598298 5.057559
H 2.411730 0.175431 3.371180
H 0.454467 2.065314 4.795099
H 1.940899 2.587830 4.003847
H 0.298090 3.014340 2.395064
H 1.151631 1.620553 1.832095
H -1.676063 1.845464 1.973813
H -1.323578 0.794059 3.379152
P 1.480477 -0.128216 -0.967883
C 2.838361 1.099306 -1.048522
C 3.156429 1.822876 -2.209561
C 4.175439 2.780486 -2.185834
C 4.893065 3.017931 -1.009661
C 4.594623 2.289323 0.147024
C 3.571512 1.339176 0.128153
H 3.339966 0.782084 1.039885
H 5.154677 2.466295 1.068427
H 5.687560 3.768050 -0.994819
H 4.411706 3.340792 -3.093855
H 2.615820 1.647874 -3.141771
C 2.306783 -1.731247 -1.317410
C 3.669852 -1.832723 -1.629288
C 4.275162 -3.080000 -1.810030
C 3.512837 -4.240641 -1.673850
C 2.150496 -4.168018 -1.363578
C 1.545544 -2.917294 -1.186772
O 0.229066 -2.747428 -0.887222
C -0.632064 -3.876098 -0.819465
H -1.642727 -3.486488 -0.644611
H -0.625282 -4.441732 -1.766765
H -0.354084 -4.548311 0.009334
H 1.572415 -5.086094 -1.261710
H 3.976173 -5.220975 -1.809623
H 5.337713 -3.139944 -2.054658
H 4.269191 -0.925912 -1.729928
C 0.389951 0.251136 -2.438065
C -1.034529 -0.298818 -2.287111
P -1.792661 0.100496 -0.628132
C -3.233805 -1.012108 -0.471089
C -3.791555 -1.175573 0.809266
C -4.894871 -2.010460 0.995244
C -5.446972 -2.696397 -0.092197
C -4.898024 -2.537768 -1.368120
C -3.797714 -1.696270 -1.561357
H -3.393014 -1.578766 -2.568339
H -5.329709 -3.067638 -2.220815
H -6.306580 -3.354803 0.055035
H -5.320821 -2.131236 1.994172
H -3.354211 -0.650243 1.661208
C -2.509242 1.778095 -0.832093
C -3.872335 1.983226 -1.085594
C -4.389848 3.272997 -1.233363
C -3.535347 4.370632 -1.126546
C -2.172207 4.193189 -0.868061
C -1.655617 2.900096 -0.714130
O -0.342827 2.638440 -0.451360
C 0.577656 3.717761 -0.340019
H 0.281107 4.421281 0.454882
H 0.670696 4.261402 -1.295289
H 1.546344 3.275150 -0.084917
H -1.524823 5.065614 -0.789187
H -3.926634 5.384344 -1.242397
H -5.454413 3.415252 -1.430378
H -4.540182 1.123069 -1.164626
H -1.681629 0.101266 -3.082596
H -1.030555 -1.394002 -2.364168
H 0.365110 1.348119 -2.507853
H 0.854753 -0.137458 -3.356836

^{4}10B-19
Geometry with 85 atoms:
Total energy: -3274.525388090
Cr -0.721934 -1.091326 0.446933
C -0.804157 -2.487090 -1.077364
C -0.225421 -3.859078 -0.698488
C -0.696996 -4.343242 0.676496
C -0.087083 -3.562887 1.844708
C -0.816333 -3.681063 3.183077
H -0.759736 -4.736446 3.503294
H -0.257897 -3.106725 3.944266
C -2.287557 -3.239399 3.201767
C -2.578824 -1.775522 2.828747
C -2.574736 -1.412223 1.332942
H -3.139366 -2.159581 0.748697
H -3.114041 -0.455824 1.208093
H -3.579799 -1.537132 3.236181
H -1.890681 -1.118618 3.395061
H -2.660489 -3.416030 4.224825
H -2.888901 -3.899604 2.553191
H 0.024934 -2.468911 1.611725
H 0.969435 -3.855773 1.970174
H -0.445251 -5.407976 0.820419
H -1.795615 -4.279200 0.711981
H 0.877622 -3.834160 -0.720558
H -0.515083 -4.608886 -1.458681
H -1.881883 -2.582833 -1.297245
H -0.320951 -2.111734 -1.997438
P 1.534355 -0.019611 -0.502461
C 2.133735 1.498804 0.348156
C 3.062514 1.365130 1.395881
C 3.478164 2.482319 2.123474
C 2.968983 3.750303 1.820269
C 2.048132 3.892033 0.779027
C 1.633484 2.775219 0.046369
H 0.911782 2.917995 -0.757243
H 1.644743 4.876826 0.531215
H 3.293974 4.624291 2.390018
H 4.206842 2.362686 2.929427

H 3.474362 0.382470 1.640504
C 3.065344 -0.988834 -0.744229
C 3.156630 -2.266600 -0.175795
C 4.323719 -3.028304 -0.279320
C 5.420512 -2.497853 -0.960224
C 5.364399 -1.220817 -1.527745
C 4.192174 -0.457187 -1.422979
O 4.058250 0.788518 -1.926927
C 5.178460 1.457557 -2.484849
H 4.832623 2.465703 -2.749114
H 6.002454 1.540571 -1.755552
H 5.544171 0.952810 -3.395727
H 6.236331 -0.827507 -2.049933
H 6.341322 -3.079263 -1.052921
H 4.373470 -4.023166 0.167731
H 2.296887 -2.667511 0.362313
C 1.016371 0.516654 -2.215176
C -0.397317 1.119907 -2.341088
P -1.586843 0.611718 -0.990191
C -3.207514 0.324703 -1.774986
C -3.270536 -0.477894 -2.928988
C -4.506507 -0.808584 -3.488032
C -5.689842 -0.353929 -2.897201
C -5.633319 0.428446 -1.740284
C -4.400209 0.764669 -1.175590
H -4.372767 1.371212 -0.268746
H -6.554568 0.780356 -1.269867
H -6.655902 -0.613916 -3.336538
H -4.543729 -1.428606 -4.386924
H -2.359075 -0.860144 -3.394637
C -1.749108 2.063789 0.106100
C -2.336248 3.261706 -0.331312
C -2.432936 4.365572 0.515654
C -1.940188 4.269756 1.820084
C -1.343941 3.092397 2.277481
C -1.236936 1.990775 1.419958
O -0.619536 0.821175 1.797970
C 0.083221 0.773099 3.045560
H -0.616701 0.835337 3.892357
H 0.831006 1.577016 3.101045
H 0.599591 -0.194634 3.073616
H -0.959730 3.049234 3.295242
H -2.015840 5.122944 2.498441
H -2.895612 5.289856 0.163974
H -2.733716 3.321191 -1.347817
H -0.369968 2.219410 -2.329107
H -0.843887 0.836851 -3.304703
H 1.773001 1.200810 -2.620156
H 1.079868 -0.414697 -2.798446

^{4}10B-20
Geometry with 85 atoms:
Total energy: -3274.523999000
Cr 0.011975 -0.645698 -0.766095
C 1.386310 -1.831402 -1.813981
C 1.518506 -3.359637 -1.667715
C 0.815320 -4.191152 -2.752567
C -0.660599 -3.848414 -2.963073
C -1.548038 -3.978234 -1.716662
H -1.710005 -5.050349 -1.508379
H -1.024720 -3.577526 -0.833286
C -2.896732 -3.249276 -1.856185
C -2.917493 -1.809357 -1.312319
C -1.798452 -0.869693 -1.793293
H -1.519180 -1.118298 -2.829733
H -2.174809 0.168781 -1.826505
H -3.898741 -1.372191 -1.578102
H -2.928677 -1.861946 -0.210391
H -3.687014 -3.815261 -1.333859
H -3.191751 -3.242150 -2.921461
H -1.075944 -4.487886 -3.761942
H -0.727853 -2.821669 -3.351113
H 0.918672 -5.262361 -2.499596
H 1.346462 -4.052094 -3.711484
H 1.150820 -3.701489 -0.687707
H 2.587916 -3.640135 -1.671447
H 1.199508 -1.571061 -2.871947
H 2.349789 -1.353222 -1.560483
P -1.273616 0.915811 0.893938
C -2.639207 2.029108 0.415685
C -2.415154 3.407840 0.248071
C -3.428171 4.232896 -0.248198
C -4.671379 3.694628 -0.592298
C -4.897174 2.322675 -0.442008
C -3.889468 1.492648 0.053147
H -4.080378 0.423257 0.157011
H -5.864115 1.891949 -0.713207
H -5.461875 4.342158 -0.979200
H -3.241619 5.303253 -0.365530
H -1.450201 3.854080 0.495909
C -2.006908 -0.410087 1.928488
C -3.110281 -0.219853 2.776880
C -3.659941 -1.288484 3.486477
C -3.112911 -2.568098 3.349460
C -2.012629 -2.781313 2.516190
C -1.465643 -1.703533 1.817575
O -0.356949 -1.894317 0.989157
C 0.731833 -2.640284 1.585171
H 0.534695 -3.719274 1.533274
H 1.638772 -2.404551 1.019876
H 0.854581 -2.333293 2.634154
H -1.595052 -3.781925 2.398986
H -3.547308 -3.412348 3.889713
H -4.519125 -1.124345 4.140233
H -3.549808 0.775932 2.870445
C -0.194032 1.872103 2.076078
C 1.138471 1.146023 2.294634
P 1.823809 0.539065 0.668012
C 3.552156 0.059247 1.006912
C 4.475080 0.031401 -0.055600
C 5.777152 -0.425616 0.155176
C 6.172646 -0.866681 1.422800
C 5.260328 -0.845918 2.481398
C 3.955295 -0.387211 2.277831
H 3.260807 -0.376221 3.120857
H 5.565023 -1.184227 3.474910
H 7.192330 -1.224069 1.584881
H 6.487504 -0.435980 -0.675134
H 4.180300 0.379133 -1.049045
C 1.921244 2.081594 -0.317358
C 2.601143 3.212980 0.162450
C 2.578602 4.419682 -0.535300
C 1.857476 4.501922 -1.729495
C 1.182518 3.389070 -2.236102
C 1.222800 2.174013 -1.538944
O 0.584535 1.040315 -2.027679
C 0.232223 1.030754 -3.428191
H -0.002737 -0.003221 -3.690693
H 1.087535 1.371705 -4.028652
H -0.648998 1.663135 -3.606794
H 0.628753 3.482590 -3.168475
H 1.817890 5.442730 -2.283534
H 3.114908 5.289364 -0.150167
H 3.157698 3.138101 1.100473
H 1.865137 1.803138 2.797056
H 1.000000 0.262606 2.938772
H -0.006625 2.855002 1.618697
H -0.722859 2.039744 3.027039